# SIDS Initial Assessment Report

# For

# SIAM 22

Paris, France, 18 – 21 April 2006

# TOME 2: SIDS Dossiers

**Category Name** **Long Chain Alcohols**

(C6-22 primary aliphatic alcohols)

| **1. and 2. Chemical Names and CAS numbers** | **CAS no.** | **Chemical name** |
|---|---|---|
| | 111-27-3 | 1-Hexanol |
| | 111-87-5 | 1-Octanol |
| | 112-30-1 | 1-Decanol |
| | 112-42-5 | 1-Undecanol |
| | 112-70-9 | 1-Tridecanol |
| | 112-72-1 | 1-Tetradecanol |
| | 629-76-5 | 1-Pentadecanol |
| | 36653-82-4 | 1-Hexadecanol |
| | 143-28-2 | 9-Octadecen-1-ol, (9Z)- |
| | 629-96-9 | 1-Eicosanol |
| | 661-19-8 | 1-Docosanol |
| | 63393-82-8 | Alcohols, C12-15 |
| | 66455-17-2 | Alcohols, C9-11 |
| | 67762-25-8 | Alcohols, C12-18 |
| | 67762-27-0 | Alcohols, C16-18 |
| | 67762-30-5 | Alcohols, C14-18 |
| | 67762-41-8 | Alcohols, C10-16 |
| | 68551-07-5 | Alcohols, C8-18 |
| | 68002-94-8 | Alcohols, C16-18 and C18 Unsaturated |
| | 68155-00-0 | Alcohols, C14-18 and C16-18-unsatd. |
| | 68333-80-2 | Alcohols, C14-16 |
| | 68603-15-6 | Alcohols, C6-12 |
| | 68855-56-1 | Alcohols, C12-16 |
| | 75782-86-4 | Alcohols, C12-13 |
| | 75782-87-5 | Alcohols, C14-15 |
| | 80206-82-2 | Alcohols, C12-14 |
| | 85566-12-7 | Alcohols, C8-10 |
| | 85665-26-5 | Alcohols, C10-12 |
| | 97552-91-5 | Alcohols, C18-22 |
| | 90583-91-8 | Tridecanol, branched and linear |

**3. Sponsor Country:** United Kingdom

**4. Shared Partnership with:**

**5. Roles/Responsibilities of the Partners:**

- Name of industry sponsor /consortium: Global ICCA Aliphatic Alcohols Consortium
- Process used: The robust summaries were prepared by contractors to the Global ICCA Aliphatic Alcohols Consortium (GIAAC). The data matrix, SIAR and IUCLID dossiers were prepared by Shell Chemicals Ltd and a contractor, Peter Fisk Associates.

**6. Sponsorship History**

- How was the chemical or category brought into the OECD HPV Chemicals Programme ?

**7. Review Process Prior to the SIAM:** All information was reviewed by the Global ICCA Aliphatic Alcohols Consortium. UK government (the Environment Agency of England and Wales, and MRC Institute for Environment and Health) peer-reviewed the SIDS documents, and audited selected key studies to check the robust study summaries.

**8. Quality check process:**

**9. Date of Submission:**

**10. Date of last Update:**

**11. Comments:** SIDS dossiers already existed for 1-Dodecanol (CAS 112-53-8) and 1-Octadecanol (CAS 112-92-5) (published in 1998 and 1995 respectively); the present document updates and extends the earlier ones; brings in new information, and therefore replaces it. No conclusions drawn in the earlier review are amended.

Available data for these substances are compiled in SIDS dossiers related to each CAS number. The reliability of each data point has been considered during this period of review, in accordance with the guidance of the Fraunhofer Institut für Toxikologie und Aerosolforschung. The following standard reliability codes, defined by Klimisch *et al.* (1997)[1], apply, in accordance with the SIDS guidance:

(1) Valid without restriction
(2) Valid with restrictions
(3) Invalid
(4) Not assignable.

Results considered to be Invalid are not used in the discussions or conclusions in this report. However, results which are of Non-assignable reliability may be fully valid, although

[1] Klimisch, HJ, Andreae, E and Tillmann, U 1997. A systematic approach for evaluating the quality of experimental and ecotoxicological data. Reg.Tox. and Pharm. 25:1-5

insufficient details were available to be sure of this; therefore reliability (4) results are used in this report. The reliability code of each data point is given.

Key studies are flagged in the SIDS dossiers. These are studies with the highest reliability/adequacy. If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/$EC_{50}$ or NOEC/ NOAEL has been indicated as the key study. For some endpoints, fully reliable results are not available and it has been necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier have been transferred from the previously published version of IUCLID or from the previous SIDS submission. In some cases, it has not been possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier. Such results are clearly identified in the SIDS dossier and more details are given therein.

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 111-27-3 |
| **CAS No.** | 111-27-3 |
| **EINECS Name** | hexan-1-ol |
| **EC No.** | 203-852-3 |
| **Molecular Formula** | C6H14O |
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **111** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491 828557

11-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC

**Remark:** Industry Consortium member
19-DEC-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** West Lathrop Avenue P.O. Box 2668
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B 1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome Minato-ku
**Town:** 100-0005 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** 1-8, 2-Chome, Bingo-Machi
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter and Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy S.p.A.
**Contact Person:** Enrico Dallara **Date:**
**Street:** V. Medici del Vascello, 26
**Town:** 20057 20138 Milano
**Country:** Italy

**Remark:** Consortium Member
09-SEP-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079-2990 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Olefins and Surfactants GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** Paul-Baumann-Strasse, 1
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK and USA
21-DEC-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
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| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |

| | |
|---|---|
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

Remark 2:

If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

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06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

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02-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Hexanol
**Smiles Code:** OCCCCCC
**Mol. Formula:** C6 H14 O1
**Mol. Weight:** 102.18

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-hexanol, CAS 111-27-3 are 100% linear.

The substance comprises >95% C6. Components of even chain length, in the range C6-C10 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required.
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Hexanol (9CI) (CA INDEX NAME)
Hexyl alcohol (8CI)
NSC 9254
Pentylcarbinol
Hexanol
Hexan-1-ol
Alcohol C-6
Caproic alcohol
Some commercial products with the name Alfol
Some commercial products with the name Lorol
1-Hexyl alcohol
1-Hydroxyhexane
Amylcarbinol
Caproyl alcohol
Epal 6
Hexanol
n-Hexan-1-ol
n-Hexanol
n-Hexyl alcohol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website
21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-hexanol.

Composition is described in section 1.1.1, General Substance Information.
05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 7000 tonnes, consumption 13 000 tonnes (alcohols in range C6-11). This is publicly-available CEH data for Japan, for 2001.

21-DEC-2005 (6) (37) (72)

## 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

## 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

## 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

## 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 26 Food/feedstuff additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Paints, lacquers and varnishes
19-SEP-2005

**Use category:** 38 Plant protection products, agricultural
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 125.
05-AUG-2005 (79)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

**CAS-No:** 111-27-3
**EC-No:** 203-852-3
**EINECS-Name:** hexan-1-ol

05-AUG-2005

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-hexanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7
02-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
11-AUG-2003

## 2.1 Melting Point

**Value:** = -44 - -51 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
31-DEC-2004 (77)

**Value:** = -51.6 degree C

**Method:** other: not specified
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. (Reference: Registry of Toxic Effects of Chemical Substances)
03-JAN-2005

## 2.2 Boiling Point

**Value:** = 158 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (77)

**Value:** = 145 - 160 degree C

**Method:** other: DIN 51751
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (40)

**Value:** = 150 - 170 degree C

**Method:** other: ASTM-D-1078
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (35)

**Value:** = 152 - 162 degree C

**Method:** other: ASTM-D-1078
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (42)

**Value:** = 157 degree C

**Method:** other: not specified
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (51)

## 2.3 Density

**Value:** = .82

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Chemfinder
**Reliability:** (4) not assignable
This value was obtained from secondary literature.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (27)

**Type:** density
**Value:** = .81 - .82 g/cm³ at 20 degree C

**Method:** other: DIN 51757 B
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.

03-JAN-2005 (40)

**Type:** density
**Value:** = 817 - 821 g/cm³ at 20 degree C

**Method:** other: DIN 51757
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (35)

## 2.3.1 Granulometry

**Remark:** Not a required OECD or HPV endpoint.
07-MAR-2000

## 2.4 Vapour Pressure

**Value:** = 1.22 hPa at 25 degree C

**Method:** other (measured)
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (18)

**Value:** = 1.21 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
valid with restrictions.

The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
11-OCT-2005 (1)

**Value:** = 1 hPa at 20 degree C

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
11-OCT-2005 (35)

**Value:** = 1.3 hPa at 20 degree C

**Method:** other (calculated)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (77)

**Value:** ca. 2 hPa at 40 degree C

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
11-OCT-2005 (40)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 2.03

**Method:** other (measured)
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The generator column was coated with liquid solute and 1-octanol. Water was then pumped into the column. Analysis of the aqueous phase from the 1% octanol coated column was used to determine the Kow.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (70)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 5900 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions

Value obtained from a recognised source of physico-chemical data. This reference is considered authoritative for water solubility values.
**Flag:** Critical study for SIDS endpoint
08-AUG-2005 (83)

**Solubility in:** Water
**Value:** = 4231 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A generator column was coated with liquid solute. Water was pumped into the column. Analysis of the aqueous phase from the pure solute coated column yielded the aqueous solubility.
**Reliability:** (2) valid with restrictions
03-JAN-2005 (70)

**Solubility in:** Water
**Value:** = 6 g/l at 25 degree C

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (36)

**Solubility in:** Water
**Value:** = 6270 mg/l at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
21-SEP-2005 (75)

**Solubility in:** Water
**Value:** = 5760 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The water solubility is estimated to be 5760 mg/l at a loading rate of 10000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
09-AUG-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 65 degree C
**Type:** closed cup

**Method:** other: DIN 51758/ISO 2719 (According to Pensky-Martens)
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (40)

**Value:** = 60 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated
03-JAN-2005 (27)

**Value:** = 62 degree C
**Type:** open cup

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (53)

**Value:** = 62 degree C

**Method:** other: DIN 51755
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (35)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Method:** Directive 84/449/EEC, A.13 "Flammability (solids and liquids)"
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
03-JAN-2005

## 2.10 Explosive Properties

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No explosive properties.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.11 Oxidizing Properties

**Remark:** No oxidizing properties.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

### 3.1.1 Photodegradation

**Method:** other (measured): method not stated
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Measured rate constant: 12.5E-12 cm3/molecule.sec
Half-life: 30.8 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of atmospheric degradation data.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (33)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
10-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 102.2
Data temperature 25 deg C
Log Kow 2.03
Water Solubility 5900 mg/l
Vapour pressure 122 Pa
Melting point -50 deg C
half life in air 30.8 h

half life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 28% |
| Soil | 6.23% |
| Water | 65.6% |
| Fish | 3.52E-04% |
| Sediment | 0.14% |

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 66.8 | 0.0375 | 0.0379 |
| % in water | 8.11 | 99.9 | 14.6 |
| % in sediment | 0.00728 | 0.0897 | 0.0131 |
| % in soil | 25.1 | 0.0141 | 85.3 |

The results reflect that the ultimate fate of 1-hexanol is dependent on its route of release into the environment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance.

The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 2.03 was used in the TGD calculation methods.

**Result:**

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 56 |
| TGD Hydrophobics method: | Koc = 118 |
| TGD Alcohols method: | Koc = 19.6 |
| SRC PCKOCWIN method: | Koc = 8.3 |

**Test substance:** As prescribed in section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods
28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 2 mg/l related to Test substance
5 mg/l related to Test substance
**Contact time:** 30 day(s)
**Degradation:** = 77 - 61 % after 30 day(s)
**Result:** readily biodegradable
**Kinetic:** 5 day(s) = 52 %
15 day(s) = 75 - 62 %
30 day(s) = 77 - 61 %
**Control Subst.:** other: Dodecylsulfate

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1988
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The first value cited in the degradation and kinetic sections is for the 2 mg/l concentration while the second value is for the 5 mg/l concentration. Due to the low solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. Although the present study does not include proof of the inertness, other studies from the same laboratory confirm this statement. The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l at the lower test concentration. At the higher test concentration, the reported dissolved oxygen concentration was below 0.5 mg/l from Day 15 onwards.
**Result:** Kinetic of control substance: 5 days = 72%
15 days = 91%
30 days = 87%
The substance degraded >60% during the 10 day window and can be regarded as readily biodegradable.
**Test condition:** Concentration of inoculum: 1 ml/l (about 10E3 - 10E5 cells/ml)
Test volume: 290-296 ml
Temperature: 20 C
pH: not reported
**Reliability:** (2) valid with restrictions
The test was not conducted to GLP and did not meet one of the validity criteria for the test at the higher test concentration.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (52)

**Type:** aerobic
**Inoculum:** other: no details provided on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 58 % after 31 day(s)

**Result:** inherently biodegradable
**Kinetic:**
4 day(s) = 35 %
10 day(s) = 49 %
17 day(s) = 55 %
24 day(s) = 57 %
31 day(s) = 58 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The inoculum used was activated sludge from a semi-continuous colony maintained in the laboratory. Incubation was carried out at 25°C in 200 ml Erlenmeyer flasks containing 5 ul of a alcohol and 100 ml of culture medium. Biodegradation rate constant was determined by measurement ofthe alcohol concentration in the supernatant of the culture by gas chromatography.
**Remark:** There is no information given on the validity criteria.
**Result:** Kinetic of control substance: 4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation during the 10 day window. Sodium Benzoate was used as a positive control and reached a mineralization extent of 62.2%.
**Test substance:** The substance corresponds to CAS# 111-27-3.
**Reliability:** (4) not assignable
Non-guideline study.
17-OCT-2005 (78)

**Type:** aerobic
**Inoculum:** activated sludge

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Incubation was carried out in 200 ml Erlenmeyer flasks containing 5 microlitres of alcohol and 100 ml of medium. Biodegradation rate constant was calculated from the time-course of the alcohol concentration in the supernatant of the culture. The concentration was analysed by gas chromatography.
**Result:** The biodegradation rate constant for Hexanol was 0.0799 hr-1. This equates to a half-life of 8.7 hours.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and more detailed data are available.
09-SEP-2005 (84)

**Type:** aerobic
**Inoculum:** other bacteria: municipal sewage treatment plant effluent
**Concentration:** 2 mg/l related to Test substance

**Degradation:** = 77 % after 30 day(s)
**Result:** readily biodegradable

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Lorol C6
**Source:** Henkel KGaA.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4.
10-JAN-2005 (24)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**GLP:** no data
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.
BOD was determined by measurement of dissolved oxygen concentrations in the test vessels at the start and end of the test period.
**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.
**Result:** 53% degradation after 5 days (% ThOD)
**Test substance:** As prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
Non-guideline study.
11-OCT-2005 (73)

## 3.7 Bioaccumulation

**BCF:** = 11

**Method:** other: calculated (Veith et al, 1979)
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 2.03 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 97.2 - 97.5
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Two papers (Veith et al 1983 a,b) appear to report the same study altough the LC50 values differ slightly, giving the range of LC50 values shown. The focus of these papers was to describe the relationship between experimentally obtained 96-h LC50 values for fathead minnows and the n-octanol/water partition coefficient.

**Result:**
RESULTS: EXPOSED
LC50 = 97.2 - 97.5 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

**Test condition:**
TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5

Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test, although analysis results were not provided.

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (75) (76)

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 117 - 126
**Limit Test:** no

**Method:** other: ASTM 1980
**Year:** 1985
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Flow-through toxicity tests were conducted with a geometric series (0.8 dilution factor) of toxicant concentrations for all tests. Test water was maintained at 25 C and pH 7.6. Successive batches of five fry or juveniles were added to each treatment and control chamber, providing a total of 20 test organisms per treatment level.
The test was performed in 1985.

**Result:** RESULTS: EXPOSED
LC50 = 126 mg/l for fry
LC50 = 117 mg/l for juveniles
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: No control mortality in tests with juveniles and less than 10% in tests with fry (refers to all 27 chemicals tested in study)

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available
19-JUL-2005 (16)

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC0:** = 30
**LC50:** = 55
**LC100:** = 100
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste

water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
**Remark:** Static exposures. Endpoint was mortality. This information is from a 1 page summary of the full report but an OECD standard method was used. 10 animals per concentration. Test was carried out prior to 1999.
**Reliability:** (2) valid with restrictions Not key study: Other studies (same reliability score) showing lesser toxicity but carried out under flow-through conditions and using measured concentrations are available
10-AUG-2005 (26)

**Type:** static
**Species:** Alburnus alburnus (Fish, estuary)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 120
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Fish from the Baltic Sea were placed into glass tanks containing water in groups of ten. The alcohol was then added to the tanks in a logarithmic series. This entry was originally reported in Linden et al 1979. However, the later report (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Result:** RESULTS: EXPOSED LC50 = 120 mg/l Based on nominal concentrations RESULTS: CONTROL Number/% showing adverse effects: not reported
**Reliability:** (2) valid with restrictions Not key study: Other studies (same reliability score) but showing greater toxicity are available
19-JUL-2005 (9) (34)

**Type:** static
**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 144

**Method:** other: not specified
**Year:** 1982
**GLP:** no data

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
20-OCT-2005 (80)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 63.4 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC0:** = 152
**EC50:** = 201
**EC100:** = 270
**Limit Test:** no

**Method:** other
**Year:** 1982
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
EC0: 152 mg/l
EC50: 201 mg/l
E100: 270 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24hrs old
Feeding: Dry algae
Pretreatment: None
Feeding during test: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none

STABILITY OF THE TEST CHEMICAL SOLUTIONS: no analysis
DILUTION WATER
Source: Standardised synthetic fresh water
Aeration: None
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Range of test concentrations to achieve three or more responses between 0 and 100%
Renewal of test solution: none
Exposure vessel type: 50 ml flask
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: oxygen saturated
pH mean: 7.6 - 7.7
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 9 hours artificial lighting
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:
None

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-JUL-2005 (15)

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 317
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available
19-JUL-2005 (9) (34)

**Type:** static
**Species:** other: tubifex tubifex (Oligochaeta)
**Exposure period:** 3 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 110
**Limit Test:** no

**Method:** other
**Year:** 1997
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Test media were prepared by dilution of a stock solution. The acute immobilisation test was carried out under static conditions. The EC50 was based on counting the number of worms that stopped moving within 3 minutes of exposure to test medium.
**Reliability:** (4) not assignable
Documentation insufficient for assessment. Information obtained from the open literature. Only a brief description of the test method is given.
20-OCT-2005 (56)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 123.6 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Selenastrum capricornutum (Algae)
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** = 11.3
**LOEC:** = 31.2
**EC10:** = 19.8
**EC50:** = 79.7
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2005
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Test condition:
TEST ORGANISMS
Strain: Pseudokirchneriella subcapitata
Source/Supplier: SAG, Culture Collection of Algae at Pflanzenphysiologisches Institut of the University at Göttingen, Albrecht von Haller Institut, Untere Klarspüle 2, D-37073 Göttingen, Catalog No 61.81.

Pretreatment: The stock cultures were maintained fulfilling the criteria of the OECD guidelines. Prior to testing a pre-culture was established in test medium to obtain exponentially growing algae for the test.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
A stock solution was prepared by adding 180 mg of the test substance to sterilized test medium and adjusting the volume to 1 L. The solution was stirred for 24 hours. The highest test concentration was diluted with sterilized growth medium to obtain the other four nominal test concentrations under sterile conditions: 7.7, 17, 37, 82 and 180 mg hexanol/L.

ANALYSIS OF EXPOSURE CONCENTRATIONS
Samples of fresh and old test media, with and without algae present were analysed to determine the concentration of the test substance. The analyte was extracted from the algae test samples by liquid-liquid partitioning with n-hexane. After shaking and settling the n-hexane extract was removed and the analyte derivatized using MSTFA. Measurement was performed by GC-MS in SIM mode using internal standard calibration with deuterated n-hexanol as internal standard.

STABILITY OF TEST CHEMICAL SOLUTIONS
The mean measured test concentrations varied in some cases by more than +/-20% of the nominal values. The results are therefore interpreted with respect to the mean measured values.

DILUTION WATER
Source: A sterilized synthetic growth medium according to OECD 201
Aeration: None reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported

TEST SYSTEM
Concentrations: 7.7, 17, 37, 82 and 180 mg hexanol/L (nominal), 4.72, 11.3, 31.2, 50.1 and 111.2 mg/L (mean measured with algae present), 5.48, 12.3, 29.3, 54.9 and 105.5 mg/L (mean measured without algae present)
Renewal of test solution: None
Exposure vessel type: Test vessels are 250 mL conical glass flasks covered with silicone-sponge caps. The vessels and caps were sterilized prior to use (autoclaving or heating). The cultures were resuspended continuously by shaking on a laboratory shaker (Incubation Shaker Multitron ®, INFORS, Switzerland).
Number of replicates: Controls: Six replicate control cultures containing only culture medium and algal suspension under sterile conditions. Three replicates of each test

concentration.
Initial cell concentration: 10,000 cells/mL.
Test temperature: 22.0 - 22.2 °C
Dissolved oxygen: Not reported
pH: 8.52 - 8.58 (Controls), 8.08 - 8.40 (testconcentrations)
Intensity of irradiation: 8000 Lux
Photoperiod: Exposed to constant lighting.

TEST PARAMETER:
End point: Growth measured as changes in cell number that were subsequently analysed with respect to growth rate and biomass.
Method of measurement: Cell concentrations were determined using an electronic particle counter (CASY 1 Model TT, Schärfe System, Reutlingen, Germany). The correctness of the electronic counts was checked by microscopically counting following internal standard operation procedures

**Result:** Based on mean measured exposure concentrations
EbC10: = 4.97
EbC50: = 20.5
LOEC: = <4.72
NOEC: = <4.72

**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (81)

**Species:** Microcystis aeruginosa (Algae, blue, cyanobacteria)
**Endpoint:** biomass
**Exposure period:** 8 day(s)
**Unit:** mg/l **Analytical monitoring:** no data
**Toxicity Threshold (TT) :**
= 12
**Limit Test:** no

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Tested in cell multiplication inhibition test. Adjustment of pH to neutral if needed. The concentration of the algal suspension of each test culture was measured turbidimetrically and expressed as the extinction of the primary light of the monochromatic radiation at 578 nm for a 10 mm layer. Control cultures were also monitored over the 8-day period.

Toxicity threshold (TT) is the pollutant concentration causing the onset of cell multiplication inhibition.

**Result:** RESULTS: EXPOSED
TT = 12 mg/l
Based on measured results

**Test condition:** TEST ORGANISMS
Strain: Microcystis aeruginosa
Supplier: Not reported
Pretreatment: None
Controls: 12 control cultures containing algal suspension, stock nutrient solution and bidistilled water under sterile conditions
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: Not reported

Vehicle, solvent: Not reported
Concentration of vehicle, solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Standard algal medium
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Not reported
Renewal of test solution: Not reported
Exposure vessel type: Culture tubes stoppered with cotton-lined metal caps
Number of replicates: 3
Initial cell concentration: Quantity of cell material used for inoculation is determined turbidimetrically and is standardised.
Test temperature: 27 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: To neutral if required
Intensity of irradiation: Not reported
Photoperiod: Exposed to constant lighting by luminescent tubes (Osram L 40/30)2 in a central field between two lateral luminescent tubes at 60 cm distance from each other.
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

**Reliability:** (3) invalid
11-OCT-2005 (13)

**Species:** Scenedesmus quadricauda (Algae)
**Endpoint:** biomass
**Exposure period:** 8 day(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT :** = 30
**Limit Test:** no

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with higher toxicity values are available.
29-DEC-2005 (12) (14)

**Species:** Euglena sp. (Algae)
**Endpoint:** growth rate
**Exposure period:** 7 day(s)
**Unit:** mg/l **Analytical monitoring:**
**LOEC:** = 75

**Method:** other: not specified
**Year:** 1980
**GLP:** no data

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
20-OCT-2005 (11)

**Species:** Scenedesmus quadricauda (Algae)
**Endpoint:** growth rate
**Exposure period:** 7 day(s)
**Unit:** mg/l **Analytical monitoring:** no
**LOEC:** = 30

**Method:** other: not specified
**Year:** 1980
**GLP:** no data

**Remark:** This is the concentration in which a 3% in extinction value occurred.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
20-OCT-2005 (11) (14)

**Species:** other algae: Chilomonas paramecium
**Endpoint:** growth rate
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LOEC:** = 18

**Method:** other: not specified
**Year:** 1980
**GLP:** no data

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
20-OCT-2005 (11)

**Species:** other algae: Enteromorpha intestinalis
**Endpoint:** other: ion retention
**Exposure period:** 2 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 400

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Samples of E. intestinalis comprising several pieces of thallus from different specimens (total weight 1 g) were risnsed once in distilled water for 3 seconds then placed in

50 ml of distilled water in a beaker and left for 2 min (sample 1). The E. intestinalis was then transferred to lidded bottles containing a further 50 ml of distilled water then placed in a boiling water bath. After 5 min the bottles were removed from the bath and the contents poured through a plastic sieve into a 100 ml beaker (sample 2). The alga was discarded. The conductivity of samples 1 and 2 was measured and used to derive an ion retention health index. This index reflects the proportion of the total leechable ions present in the thallus which were retained after exposure to distilled water for 2 mins. The index was calculated by dividing the conductivity of sample 2 by the total conductivity (i.e. sample 1 + sample 2).

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with lower effect values are available.

20-OCT-2005 (57)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Type:** aquatic
**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 16 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT or EC3 :** = 62

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The multiplication of bacterial cells of the genus Pseudomonas is inhibited by dissolved toxic water ingredients. After a certain period the increase in the number of cells in a test culture free from toxic influence and with a standardized offer of nutrients will exceed that observed in a test culture containing dissolved toxic substances and kept under identical conditions.
The concentration of the bacterial suspension is measured turbidimetrically (while diffused light is screened off); it is expressed by the extinction of the primary light of the monochromatic radiation at 436 nm for a layer of 10 mm thickness. The concentration at which the inhibitory action of a pollutant starts will be present in that step of a dilution series of the pollutant having an extinction value at the end of the test period that is >= 3% below the mean value of extinction for non-toxic dilutions of the test cultures.

**Test condition:** TEST ORGANISMS
Supplier: Stock cultures
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: Not reported
Vehicle, solvent: Not reported
Purity/supplier: Not reported
DILUTION WATER
Source: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported

TEST SYSTEM
Concentrations: Not reported
Dosing rate: Not reported
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 25 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: None
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported

**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.

19-JUL-2005 (14)

**Species:** Uronema parduzci (Protozoa)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 93

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available

19-JUL-2005 (77)

**Species:** other protozoa: Entosiphon sulcatum
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT or EC3 :** = 75

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

19-JUL-2005 (14)

**Type:** aquatic
**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 1000
**EC10:** = 3000

**Method:** other: DIN 38412 Teil 8 (cell multiplication inhibition test)
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test substance:** Lorol C6.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is

available.
06-AUG-2005 (24)

**Type:** aquatic
**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 16 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** 3000
**EC10:** 10000

**Method:** other: DIN 38412 teil 27 (respiration inhibition test
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test substance:** Lorol C6
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
18-JAN-2006 (29)

**Type:** aquatic
**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** 300.4

**Method:** other: not specified
**Year:** 1990
**GLP:** no data
**Test substance:** no data

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
4. This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
06-AUG-2005 (58)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)
**Unit:** mg/l **Analytical monitoring:**
**NOEC:** = 6.8 - 13 calculated

**Method:** other: calculated (QSAR)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

Structure-activity relationships have been developed based on these results. It is possible to apply these structure-activity relationships to estimate chronic toxicity endpoints where there are no reliable measured data.

Two QSAR relationships have been developed. It can be concluded that the NOEC for reproduction would be within the range of the two estimates.

**Result:** It can be estimated that chronic NOEC(reproduction) for Daphnia magna would lie in the range of 6.8 - 13.0 mg/l.

**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
19-JUL-2005 (19)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:

n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.

No further information on other biotransformation pathways of these alcohols was provided.

**Source:** Kamil et al, 1953
Hayes Consultancy Service Bromley, Kent

**Test condition:** These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including the C6-C18 alcohols within this category, form glucuronic acid conjugates in the rabbit.

Groups of 3 Chinchilla rabbits, about 3 kg in weight, were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.

The results were reported as the amount of extra glucuronic acid excreted as a % of dose.

**Test substance:** n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol

**Conclusion:** All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

11-NOV-2004 (32)

**Remark:** Hexyl alcohol is oxidised to hexanoic acid which is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Test substance:** Hexanol (linear primary alcohol)

**Reliability:** (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including n-hexanol.

11-NOV-2004 (82)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: Holtzman albino
**Sex:** male/female
**No. of Animals:** 60
**Vehicle:** other: undiluted
**Doses:** 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
**Value:** = 3210 mg/kg bw

**Method:** other: not specified
**Year:** 1965
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All deaths occurred within 24 hours of dosing

- Number of deaths at each dose: 0/10, 1/10. 4/10. 4/10, 8/10, 8/10.

CLINICAL SIGNS: Animals at all dose levels exhibited weakness and ataxia. They became comatose and breathing was laboured while comatose. Animals which survived appeared normal within 24 hours other than top dose animals (6.55 g/kg) where the rats appeared unwell up to 48 hours after dosing. Weight gain amongst survivors was within normal limits.

NECROPSY FINDINGS: Necropsy of animals which died showed congestion of the lungs and adrenals in most animals. In some cases gastric congestion was also observed. There were no remarkable gross findings in animals sacrificed at the end of the observation period.

POTENTIAL TARGET ORGANS: No conclusion drawn.

SEX-SPECIFIC DIFFERENCES: None reported, mortality was presented as a combined value so no independent assessment can be made.

**Source:** Scientific Associates, Inc. 1965a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS:
- Source: No data
- Weight at study initiation: 200 - 265 g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION:
- Doses: 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
- Doses per time period: single
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during

the observation period. Body weights of survivors were recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

**Test substance:** Trade name Alfol 6

**Conclusion:** The rat oral LD50 value (M+F) for Alfol 6 was 3.21 g/kg confidence limits 2.35 to 4.39 g/kg. No specific target organ was identified.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Well documented and conducted study.

**Flag:** Critical study for SIDS endpoint

15-JUL-2005 (29) (59)

**Type:** LD50
**Species:** rat
**Strain:** other: COX-SD
**Sex:** male/female
**No. of Animals:** 50
**Vehicle:** other: undiluted
**Doses:** 2, 3.17, 5.02, 6.32 and 7.96 g/kg
**Value:** = 4420 mg/kg bw

**Method:** other: in house protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All decendents died on the day of dosing.
- Number of deaths at each dose: 0/10; 0/5M 3/5F; 2/5M 3/5F; 3/5M, 4/5F; 10/10.

Rat oral LD504.42 g/kg (confidence limits 3.95 - 4.95).

CLINICAL SIGNS: At the lowest dose (2g/kg) 6 animals showed no signs of intoxication. The 4 remaining animals and all animals at the higher dose levels showed one or more of the following: Hypoactivity, diarrhoea, hypersalivation. hyper lacrymation, haematuria, maliase, ataxia, proneness, loss of righting reflex and sedation. All survivors returned to normal between 24 and 72 hours after dosing. With the exception of 1 male at the 6,32 g/kg level which showed a poor weight gain all other survivors gained weight within expected limits.

NECROPSY FINDINGS: Animals which died prematurely showed one or more of the following gross abnormalities: moderate to severe congestion of the kidneys, adrenals, lungs, liver, stomach and gastrolintestinal tract. There was thickening (translucent portion) and erosion of the gastric mucosa.

Animals necropsied at sacrifice showed in all proliferation of the gastric mucosa (translucent portion) up to 10-90% in some rats. Also observed in some rats adhesion of the stomach to major abdominal organs and/or the abdominal wall and pallor of the pancreas. One rat showed a whitish-green kidney medulla.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: Females appear more sensitive based on mortality data.

**Source:** Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (COX-SD)
- Source: Not reported.
- Age: Not reported
- Weight at study initiation: 198-254g
- Group size: 5M+5F/group fasted
- Controls: No

ADMINISTRATION: Oral gavage
- Doses: 2, 3.17, 5.02, 6.32 and 7.96 g/kg
- Doses per time period: single
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were recorded several times on the day of dosing and thereafter daily throughout the observation period. All premature decedents and survivors were subject to gross necropsy. All surviving animals were weighed prior to sacrifice. the LD50 was calculated using the method of Litchfield and Wilcoxon, 1949.

**Test substance:** Tradename Alfol 6

**Conclusion:** The rat oral LD50 for Alfol 6 was 4.42 g/kg. The gastric mucosa appears to be a target organ.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restirictions. Well documented and well conducted study.

**Flag:** Critical study for SIDS endpoint

11-NOV-2004 (29) (62)

**Type:** LD50
**Species:** mouse
**Sex:** male/female
**Vehicle:** other: undiluted
**Doses:** not reported
**Value:** = 4000 mg/kg bw

**Method:** other
**Year:** 1963
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The mouse LD50 value for n-hexanol is 4 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain.

**Source:** Zaeva, 1963
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg). The actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination. n-hexanol was tested as part of a comparative study with other alcohols.

**Reliability:** (4) not assignable
Original document in Russian (translation available),

experimental detail limited but result considered valid.
13-OCT-2004 (48) (85)

**Type:** LD50
**Species:** rat
**Strain:** Sherman
**Sex:** male
**Vehicle:** other
**Value:** = 4590 mg/kg bw

**Method:** other: Smyth & Carpenter, 1944 & 1948
**Year:** 1951
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Rat oral LD50 4590 mg/kg (confidence limits 4030-5940 mg/kg).
**Source:** Smyth et al, 1951
**Test condition:** Groups of 6 male rats received doses of the test material at 10 fold dose intervals, followed by 2 groups of 10 rats at intermediate doses as appropriate.
**Reliability:** (4) not assignable
Summary data on a number of substances, result valid but reporting limited.
12-SEP-2004 (29) (48) (68)

**Type:** LD50
**Species:** rat
**Value:** = 4870 mg/kg bw

**Method:** other
**Year:** 1967
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Value reported in Patty 2000, no experimental details given. This value referenced to Baer & Griepentrog, 1967 which is itself a secondary reference.
**Reliability:** (4) not assignable
Secondary reference, original in German, no experimental details available.
13-OCT-2004 (48)

**Type:** LD50
**Species:** rat
**Sex:** no data
**Value:** = 3131 - 3344 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No further experimental details available. Company data reported original report unavailable.
**Test substance:** Tradename Nacol 6 RD
**Reliability:** (4) not assignable
Secondary reference
13-OCT-2004 (29)

**Type:** LD50
**Species:** mouse
**Sex:** no data
**Value:** = 1950 mg/kg bw

**Method:** other: no data
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Secondary reference
12-SEP-2004 (29) (55)

**Remark:** Several other LD50 values are reported in IUCLID 2000 ascribed to either Henkel (1) or the Dangerous Properties of Industrial Materials Report for hexanol (2).

The values are all for rats and are as follows:

LD50 4870 mg/kg and 4000 mg/kg (1)
LD50 4100 mg/kg and 4900 mg/kg (2)

No experimental details are given.
**Reliability:** (4) not assignable
Secondary references.
12-SEP-2004 (29)

### 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** other:COX-SD
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: atmosphere generated as a mist
**Doses:** 21 mg/l
**Exposure time:** 1 hour(s)
**Value:** > 21 mg/l

**Method:** other: in house protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: During exposure all animals showed hypoactivity and/or ataxia, lethargy and prostration. However within 2 hours of removal from the exposure chamber the animals all appeared and continued to appear normal throughout the observation period. Final bodyweights showed a slight weight loss in one animal however the others all exhibited weight gains within expected limits.

NECROPSY FINDINGS: Gross necropsy revealed moderate pulmonary, adrenal and hepatic congestion in one animal only. The findings in the remaining 9 test animals were unremarkable.

POTENTIAL TARGET ORGANS: None identified.

**Source:** Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

**Test substance:** Tradename Alfol 6

**Conclusion:** The rat inhalational LC50 following a 1 hour exposure to a mist of Alfol 6 was >21 mg/l.

**Test condition:** TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 245-356g
- Number of animals: 5m+5F/dose level
- Controls: none

ADMINISTRATION: inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a mist, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 0.21 mg/l for 1 hour (not monitored)
- Particle size: Droplet size not reported
- Type or preparation of particles: The mist was generated using a nebuliser.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

**Reliability:** (2) valid with restrictions
Study well documented meeting generally accepted scientific principles, acceptable for assessment. Only one dose level, short exposure period, no indication of droplet size.

**Flag:** Critical study for SIDS endpoint

12-SEP-2004 (29) (62)

**Type:** LC50
**Species:** rat
**Strain:** Sherman
**Sex:** male
**Exposure time:** 8 hour(s)

**Method:** other: screening
**Year:** 1951
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The 8 hour LC50 of n-hexanol is greater than the substantially saturated vapour concentration. No rats died during this exposure.

**Test condition:** Groups of 6 rats were exposed to the substantially saturated vapours of n-hexanol generated by passing air through a disc bubbler at room temperature for up to 8 hours. There was no measurement of vapour concentration.

**Reliability:** (4) not assignable
Summary data on a number of substances, reporting limited. No measurement of vapour concentration.

12-SEP-2004 (48) (68)

**Type:** LC50
**Species:** other: rat, mouse, guinea pig
**Value:** > 1060 ppm

**Method:** other: no data
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Secondary literature
12-SEP-2004 (46) (55)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rat
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 40
**Vehicle:** other: applied undiluted
**Doses:** 1, 2, 3 and 4 g/kg
**Value:** = 2330 mg/kg bw

**Method:** other: contract laboratory protocol
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: Deaths occurred from day one until day 10 of the observation period for both intact and abraded skin.
- Number of deaths at each dose: 0/10, 3/10, 5/10, 10/10 combined male and female mortality for intact skin. 0/10, 4/10, 8/10, 10/10 combined male and female mortality for abraded skin.

LD50(s): Intact skin M+F 2.33 g/kg (1.81-2.99) Males 2.40 g/kg (1.66-3.48) Females 2.39 g/kg (1.60-3.56). Abraded skin M+F 2.15 g/kg (1.71-2.71) Males 2.15 g/kg (1.55-2.00) Females 2.15 g/kg (1.55-2.99) Combined intact and abraded M+F 2.24 g/kg.

APPLICATION SITE: Slight to severe erythema in most animals at all dose levels, slight to servere oedema in all animals at all dose levels. At 24 hours thickening, blanching and wrinkling was also reported. Erythema and oedema persisted to 72 hours in some animals. At days 7 and 14 these changes progressed to thickening , maceration, wrinkling, dryness, coriaceousness, desquamation, sloughing and scar tissue formation.

CLINICAL SIGNS: These were reported combined for intact and abraded skin and males and females.
1 g/kg: 2/20 animals appeared thin by observation day 7. An overall weight loss was reported for 4/20 rats (1 intact skin) ranging from 0.42 (intact) to 17.36% (abraded).
2 g/kg: 15/20 showed some of the following- pallor, hypersensitivity to touch, generalised weakness, malaise, hunched position and thinness. 7/13 survivors showed a weight loss.
3g/kg: 17/20 showed some of the following: pallor, generalised weakness, hunched position, diarrhoea, hypothermia, dyspnea, thinness, prostration, moribundity. All survivors showed

either weight loss or minimal weight gain.
4 g/kg: 7/20 surivived more than 24 hours and these showed some of the following prior to death: pallor, hypersensitivity to touch, generalised weakness, hypothermia, prostration. All animals died by observation day 5.

NECROPSY FINDINGS: 1g/kg: All animals survived to the end of the observation period in 14/20 necropsy finding were unremarkable. Two animals showed accumulation of clear fluid in the peritoneal cavity, 3 pale-tan kidneys, and 3 a decrease in fatty tissue in the viscera.

2g/kg: 13 animals survived, of these necropsy findings were unremarkable in 7 rabbits. Two surviving animals had accumulation of clear fluid in the peritonal cavity, 1 severe erosion of the gastric mucosa, and 5 depletion of visceral fat. Among the 7 mortalites, 1 showed a slight accumulation of clear fluid in the peritoneal cavity, 3 severe congestion of the kidneys, 6 erosion of the gastric mucosa, 1 congestion of the lungs, 2 a friable liver, 4 depletion of visceral fat, and one post mortem autolysis of visceral organs.

3g/kg: 7 animals survived of these necropsy findings were unremarkable in 4 rabbits. In other surviving animals 1 animal with pale-tan kidneys, 1 with enlarged kidneys, 1 with a thickened stomach wall, and 1 with depletion of visceral fat. In the animals which died, 3 animals had congestion of the kidneys, 12 severe erosion of the gastric mucosa, 2 congestion of the lungs, 2 a mottled liver, 5 congestion of the small intestines, 1 congestion of the caecum, 1 reddish tinged urine , and 2 with post-mortem autolysis of the abdominal viscera.

4 g/kg: All animals died. Five animals showed congestion of the kidneys, 12 severe erosion of the gastric mucosa, 5 congestion of the lungs, 1 accumulation of fluid in thoracic cavity, 4 reddish tinged urine, and 2 post-mortem autolysis of the abdominal viscera. In one animal findings were unremarkable.

POTENTIAL TARGET ORGANS: gastric mucosa

SEX-SPECIFIC DIFFERENCES: No marked difference in LD50. Clinical signs were not reported separately.

**Source:** Scientific Associates, Inc. 1980
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3 - 3.02 kg
- Group size: 5M+5F
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2, 3 and 4 g/kg
- Removal of test substance: Excess material removed with

absobent paper towels. Attempts were made to estimate the amount of unabsorbed material but this was not possible.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation days 7 and 14. All decedents and survivors were subject to gross necropsy. The LD50 was calculated using the method of Litchfield and Wilcoxon, 1949.

**Test substance:** Tradename Alfol 6

**Conclusion:** The rabbit dermal LD50 for Alfol 6 following a 24 occluded exposure to intact skn is 2.33 g/kg. There was significant evidence of skin irritation at the application site persisting in some animals throughout the observation period. Clinical signs were indicative of a general toxic effect coupled with anorexia. The most common gross pathological finding was erosion of the gastric mucosa.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restirictions. Well documented and well conducted study not to GLP.

**Flag:** Critical study for SIDS endpoint

15-JUL-2005 (29) (63)

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: undiluted
**Doses:** 0.5, 1, 1.5 and 2 g/kg
**Value:** = 1500 - 2000 mg/kg bw

**Method:** other: contract laboratory protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: Within 48 hours of dosing.
- Number of deaths at each dose: 0/4, 1F/4, 1M/4, 4/4.

Rabbit dermal LD50 (24 hour occlusive exposure) 1.5 - 2 g/kg. This is a combined value for intact and abraded skin and males/females.

APPLICATION SITE: At 24 hours all animals showed slight to moderate erythema especially of the ventral region. Survivors all showed wrinkling and/or coriaceousness, hardening and desquamation of the skin which persisted throughout the observation period.

CLINICAL SIGNS: Prior to death generalised weakness and/or unthriftiness, diarrhoea, hypothermia, pallor, loss of corneal and palepebral reflexes, hunched position, flaccidity, slow shallow repsiration and coma. Similar signs of intoxication but less marked were observed in survivors. All survivors appeared systemically normal within 96 hours of dosing. Among survivors there was weight loss in 3 rabbits, one rabbit maintained a constant weight, while the remaining survivors

showed weight gains within expected limits.

NECROPSY FINDINGS: Premature decedents showed at gross necropsy, in addition to dermal irritation, severe haemorrhaging and/or bloody, gelatinous infiltration of the subcutis, depletion of fatty tissue, slight accumulation of clear fluid within the peritoneal cavity, moderate congestion of liver and kidneys and severe haemorrhaging and/or blanching of the gastric mucosa.

Amongst survivors (10), other than residual skin damage, gross necropsy findings were unremarkable in 7 rabbits. In the remaining 3 rabbits there was a slight to moderate accumulation of clear viscous liquid in the peritoneal cavity and/or a dpeletion of visceral fat and mottling or stippling of the renal cortex.

POTENTIAL TARGET ORGANS: None identified.
SEX-SPECIFIC DIFFERENCES: None obvious.

**Source:** Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported.
- Age: Not reported.
- Weight at study initiation: 2.3 - 2.9 kg
- Group size: 2M+2F intact and abraded skin
- Controls: None

ADMINISTRATION: 24 hour occlusive
- Area covered: Not reported.
- Occlusion: Plastic binder.
- Vehicle: Undiluted
- Doses: 0.5, 1, 1.5 and 2 g/kg
- Removal of test substance: Washing and blotting dry with paper towels.

EXAMINATIONS: The animals were observed for clinical signs of intoxication several time during the day of dosing and daily thereafter throughout the 14 day observation period. The animals were weighed at sacrifice. All premature decedents and survivors were subjected to gross necropsy.

**Test substance:** Tradename Alfol 6

**Conclusion:** The rabbit dermal 24 hour occlusive LD50 (combined applications to intact and abraded skin) is 1500-2000 mg/kg.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (small group size).

**Flag:** Critical study for SIDS endpoint

11-NOV-2004 (7) (29)

**Type:** LD50
**Species:** rabbit
**Vehicle:** other: undiluted
**Value:** = 3100 ml/kg bw

**Method:** other: Draize, 1944
**Year:** 1951
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The acute dermal LD50 for n-hexanol is reported as 3100 ml/kg (confidence limits 2020-4770) equivalent to 2530 mg/kg.
**Test condition:** The dermal toxicity of n-hexanol in the rabbit was determined using a modification of the rubber cuff method advocated by the FDA at the time of this study. The test material was applied undiluted and remained in contact with the skin under an occlusive dressing for 24 hours. Animals were then observed for 14 days and mortality recorded. No further details of group size, clinical signs etc were available.
**Reliability:** (4) not assignable
Documentation insufficient for assessment.
13-OCT-2004 (29) (48) (55) (68)
**Type:** LD50
**Value:** > 5000 mg/kg bw

**Method:** other
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The acute dermal LD50 in rabbits is reported as >5000 mg/kg.
**Reliability:** (4) not assignable
Secondary reference no experimental details given.
12-SEP-2004 (29) (46) (48)

**Remark:** Other LD50 values are reported in IUCLID 2000 ascribed to either Henkel (1) or the Dangerous Properties of Industrial Materials Report for hexanol (2).

The values are for rabbits and are as follows:

LD50 2530 mg/kg (1)
LD50 2500 mg/kg (2)

No experimental details are given.
**Reliability:** (4) not assignable
Secondary references.
12-SEP-2004 (29)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive

**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE Group mean 24+48+72 hour
- Erythema: 2.13 (72 hour score 2.2)
- Edema: 0.6 (72 hour score 0)

(individual scores were not reported) Erythema and oedema were observed at 1 hour post-exposure.

REVERSIBILITY: Oedema had reduced to 0 at 48 and 72 hours. Erythema reached a maximum of 2.2 at 48 hours persisting at this level to 72 hours.

OTHER EFFECTS: None reported

**Source:** Jacobs & Martens, 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 4 hour exposure
- Preparation of test substance: Undiluted
- Area of exposure: 6 cm2
- Occlusion: Under and exposure chamber
- Vehicle: Undiluted
- Postexposure period: 72 hours
- Removal of test substance: Not reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24 , 48 and 72 hours after end of application.

**Conclusion:** Based on a group mean 24+48+72 hour erythema score of >2 (2.13) 1-hexanol would be classified as irritant according to EU criteria. Although individual scores are not reported 6 animals were used and it is considered that 1-hexanol will be classified as a mild irritant according to GHS criteria.

Cited in Iucldi 2000

**Reliability:** (2) valid with restrictions
Guideline study without detailed documentation.

**Flag:** Critical study for SIDS endpoint
15-JUL-2005 (29) (30)

**Species:** rabbit
**Concentration:** undiluted

**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**PDII:** 3.58
**Result:** moderately irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hour
- Erythema: Intact skin 2.03, abraded skin 2.30 (72 hour score intact 2.2, abraded 2.6) Individual scores 3/6 >= 2.3 intact, 4/6 for abraded.
- Oedema: Intact skin 1.23, abraded skin 1.93 (72 hour score intact 0.7, abraded 1.3)

REVERSIBILITY: Over the observation period (72 hours) erythem increased in 4 rabbits while oedema reduced in all rabbits.

OTHER EFFECTS: At 24 and 48 hours the skin at the treatment site in 4 rabbits showed moderate to marked diffuse blanching, with a more intense reaction involving or immediately surrounding the abraded skin.

**Source:** Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour application to intact and abraded skin.
- Preparation of test substance: As a suspension.
- Area of exposure: 1 inch square
- Occlusion: Occlusive
- Vehicle: undiluted
- Postexposure period: 72 hours
- Removal of test substance: Washed off the treated skin (no further details).

EXAMINATIONS
- Scoring system: Draize et al, 1944
- Examination time points: 24, 48 and 72 hours after application.

**Test substance:** Tradename Alfol 6

**Conclusion:** Based on the erythema scores reported Alfol 6 is a skin irritant according to EU criteria. 24+48+72 hour mean score of 2.03 for intact and 2.3 for abraded skin. In the absence of information later than 72 hours post exposure Alfol is also considered an irritant according to GHS criteria.

Cited in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Standard Draize test, reasonably documented, however the test was terminated at 72 hours when there was still marked irritation.
**Flag:** Critical study for SIDS endpoint
11-NOV-2004 (29) (62)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Open
**No. of Animals:** 5

**Method:** other
**Year:** 1951
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test methods are those used in earlier publications by these workers (Smyth et al, 1944) and they are not comparable with the guideline methods currently used so the data obtained is not of great relevance. A volume of 0.01 ml was applied undiluted to the shorn belly of rabbits and was observed after 24 hours.
**Result:** The skin was reported to show a grade 3 reaction (strong capillary injection). This is described as moderate irritation in Patty, 2001 and Opdyke, 1985. The lack of individual scores and the use of a non-standard technique preclude classification on the basis of EU or GHS criteria.
**Source:** Hayes Consultancy Service Bromley, Kent
**Reliability:** (3) invalid
Invalid test method.
07-SEP-2004 (46) (48) (68)

**Species:** rabbit
**Concentration:** 6 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**Vehicle:** other: mineral oil
**PDII:** 1.16
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** other: presume Draize
**Year:** 1970
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The result of this study was reported as a primary irritation index (PII) which was 1.16. No other study details were available. A PII score of 1.16 would not trigger classification as irritant using either the EU classification system or GHS. Hexanol tested in mineral oil can therefore be considered as at most mildly irritating (GHS category 3) and non-irritant according to EU criteria.
**Source:** Procter and Gamble 1970.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain/sex/source/age/weight: not reported

- Number of animals: Not reported
- Controls: None

ADMINISTRATION/EXPOSURE
From the age of the study and the fact that it was carried out in the USA this is likely to be a Draize test with 24 hour exposure.
- Occlusion: Reported as a patch test
- Vehicle: mineral oil
- Concentration in vehicle: 6%
- Total volume applied: Not reported
- Postexposure period: Not reported

EXAMINATIONS
- Scoring system: Not reported presume Draize, results reported as PII.
- Examination time points: Not reported

**Conclusion:** From the limited data available 1-hexanol (6% in mineral oil) is not a skin irritant according to EC or GHS criteria.

**Reliability:** (4) not assignable
Documentation insufficient for assessment.

**Flag:** Critical study for SIDS endpoint

13-OCT-2004 (50)

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Occlusive
**Exposure Time:** 6 day(s)
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Result:** highly irritating

**Method:** other: repeated skin application
**Year:** 1963
**GLP:** no
**Test substance:** other TS: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

**Result:** The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol.

**Source:** Zaeva, 1963 reported in BIBRA, 1995. Clayton and Clayton, 1994.

Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental details were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol.

**Conclusion:** Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit skin for 6 consecutive days resulted in marked irritation with

eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol. Also reported by BIBRA, 1995. Clayton and Clayton, 1994.

**Reliability:** (2) valid with restrictions
Non-standard test with limited documentation. Useful for supporting information.

15-JUL-2005 (17) (85)

**Species:** other: rabbit, guineapig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: vaseline

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** other TS: even C6-22 alcohols

**Result:** The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12) to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. The human scores generally were less than those of the rabbits and reached a peak of class 3 with the C10 alcohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guinea pigs followed no obvious pattern and all scores were classed as <=3.

In some cases alcohols have been given descriptive ratings for rabbits and man in Iuclid datasets. These ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol) reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C6-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. All applications were made at a concentration of 50% in vaseline. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible. N-hexanol applied as 50% in vaseline produced practically no skin irritation in rabbits, hairless mice and human volunteers and marginal irritation in guineapigs.

Cited in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

11-NOV-2004 (29) (31)

**Species:** rabbit
**Result:** moderately irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1986
**GLP:** no data
**Test substance:** other TS: Nacol 6 RD

**Reliability:** (4) not assignable
Secondary reference to study carried out to OECD 404 for Condea Chimie GmbH, original unavailable.

13-OCT-2004 (29)

**Remark:** Cited in Iuclid 2000 as Henkel report TBD 910457 which is unavailable. Irritation study in rabbits, no further details reported. Described as moderately irritating.
**Test substance:** 1-hexanol
**Reliability:** (4) not assignable
Secondary reference.

13-OCT-2004 (29)

**Remark:** Summary data cited by RTECS obtained from Union Carbide Data Sheet, 1967. 410 mg of n-hexanol was applied to rabbit skin in an open irritation test. The degree of irritation was described as mild. No further details available, original unobtainable.
**Reliability:** (4) not assignable

Secondary reference
13-OCT-2004 (55)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** irritating
**EC classificat.:** irritating

**Method:** other: contract laboratory procedure
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE: The scores were reported as prescribed by the FDA 1965. Although individual animal data was provided only the converted scores were reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each tiem point was as follows:

1 hour: 14
24 hours: 31.8
48 hours: 37.7
72 hours: 32.4

DESCRIPTION OF LESIONS:
- Cornea: opacity (slight density and involving about half the corneal surface) in all rabbits from 24 hours after instillation. At 72 hours described as easily discernable to opalescent and involving about 1/4 to 3/4 of the corneal surface in 5/6.
- Iris: barely perceptible to minimal iritis (grade 1) in 4/6 rabbits from 24 hours after instillation. At 72 hours described as barely perceptible to slight in 3/6.
- Conjunctivae (Redness): Slight to severe conjunctivitis in all eyes from 24 hours. At 72 hours described as slight to severe in 6/6.
- Conjunctivae (Chemosis): Moderate to pronounced chemosis of the eye lids with a slight to copious watery-mucoid discharge in all animals.

REVERSIBILITY: Irritation was evident up to and including the 72 hour observation period. There was improvement in one animal, little change in 3 animals and a worsening of the condition in 2.

**Source:** Scientific Associates, Inc. 1977c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported

- Number of animals: 6
- Controls: The other eye served as control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 72 hours

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: FDA 1965
- Observation period: 1, 24, 48 and 72 hours.
- Tool used to assess score: Fluorescein

**Test substance:** Tradename Alfol 6.
**Conclusion:** Based on the descriptions of the lesions it is considered that Alfol 6 is classifiable as an irritant according to EU criteria and a class 2 irritant according to GHS.
**Reliability:** (2) valid with restrictions
Reasonably documented, however the test was terminated at 72 hours when there was still marked irritation.
**Flag:** Critical study for SIDS endpoint
11-NOV-2004 (62)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 4
**Vehicle:** none
**Result:** irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: Individual 3, 2, 2, 1.7 Mean 2.2
- Iris: Individual 2, 1, 1, 1.3 Mean 1.3
- Conjunctivae (Redness): Individual 3, 2, 3, 2.7 Mean 2.7
- Conjunctivae (Chemosis): Individual 3, 2, 3, 2 Mean 2.5
- Overall irritation score: MMAS (modified maximum score 64.8)

REVERSIBILITY: Effects on the cornea and iris had reversed by 7 days, redness and/or chemosis persisted to 7 days in one rabbits, 10 days in 2 animals and 14 days in the final rabbit, all scores were 0 by day 21.
**Source:** ECETOC, 1998
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Unspecified
- Source: No data

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 21 days

EXAMINATIONS

- Ophthalmoscopic examination: No data
- Scoring system: No data
- Observation period: 24, 48, 72 hours, 7, 10, 14 and 21 days (assessments made until the test eye for each animal showed complete reversal to normal up to 21 days)
- Tool used to assess score: No data

The study was included as part of a data base of in vivo eye irritation results. All studies were conducted to OECD guideline 405 under GLP.

**Conclusion:** 1-hexanol is classifiable as an eye irritant according to EU criteria (based on 24+48+72 hour mean scores =>2 for corneal opacity (2.2) and chemosis (2.5) and =>2.5 for conjunctival redness (2.7) reversible within 21 days. According to GHS criteria 1-hexanol is a Class 2A irritant based on individual mean 24+48+72 hour scores in at least 2 test animals of => 1 for corneal opacity and iritis and => 2 in at least 2 test animals for conjunctival chemosis and redness. Only 1 animal scored => 3 for corneal opacity or => 1.5 for iritis.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

15-JUL-2005 (20)

**Species:** rabbit
**Concentration:** undiluted
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 1.3 (96 hr 2) (opacity)
- Iris: 0.1 (96 hr 0)
- Conjunctivae (Redness): 2.5 (96 hr 1.8)
- Conjunctivae (Chemosis): 0.8 (96 hr 0)

Individual animal data were not provided.

DESCRIPTION OF LESIONS: Scores only reported no description of lesions.

REVERSIBILITY: Effects had not fully reversed over the observation period. Corneal opacity increased up to 24 hours. All other parmeters scored showed a reduction in response over 96 hours.

OTHER EFFECTS: The % surface of the cornea affected by corneal damage was reported as follows: 4 hour 77%; 24 hours 67%; 48 hour 50%; 72 hour 17%; 96 hours 0%.

**Source:** Jacobs & Martens, 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit

- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: undiluted
- Postexposure period: 96 hours

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: Draize scores at 4, 24, 48, 72 and 96 hours post exposure.
- Observation period: 96 hours
- Tool used to assess score: One drop 2% sodium fluorescein .

**Conclusion:** 1-hexanol is an eye irritant according to EU criteria with group mean 24+48+72 hour scores for conjunctival redness of 2.5. Although individual scores are not available, 6 animals were used and it is considered that 1-hexanol is a Class 2A eye irritant according to GHS criteria.

**Reliability:** (2) valid with restrictions
Guideline study without detailed documentation.

**Flag:** Critical study for SIDS endpoint

15-JUL-2005 (29) (30)

**Remark:** Reported as severely irritant to the rabbit eye using the method of Carpenter & Smyth, 1946. This method is not an accepted method for evaluation of eye irritancy and the results cannot be considered as valid.

**Source:** Smyth et al, 1951

**Test substance:** Reported as 1-hexanol.

**Reliability:** (3) invalid
Method invalid.

17-OCT-2004 (48) (68)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** other: 1 drop
**Exposure Time:** unspecified
**Comment:** no data
**No. of Animals:** 5

**Method:** other: non-standard
**Year:** 1963
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** One drop of undiluted material was instilled into the eye of 5 rabbits. No further experimental details are reported.

**Result:** All the alcohols studied caused redness and swelling of the mucous membranes of the eye. These disappeared almost completely within 4-5 hours. The most marked changes were observed with n-hexanol and are described as suppurative conjunctivitis and cloudiness of the cornea. There is no

information given on the reversibility of these changes. The results suggest that except for 1-hexanol the alcohols tested are at most slightly irritating to the eye. With no information on the reversibility of effects over time no meaningful conclusion can be drawn about the degree of eye irritation caused by 1-hexanol in this study.
**Source:** Zaeva, 1963
**Test substance:** The following alcohols were investigated in this comparative study: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol
**Reliability:** (3) invalid
Documentation insufficient for assessment.
17-OCT-2004 (85)

**Remark:** Iuclid 2000 reports (in summary) 2 eye irritation studies in rabbits with Alfol 6. Both tests are described as Draize tests. The EC classification was given as irritating in both tests although in one test the result was described as highly irritating (Scientific Assoc. 1965 for Continental Oil) and in the other moderately irritating (Hazelton Inc. 1982 for Conoco Inc). No further details are available.
**Test substance:** As prescribed. Trade name Alfol 6
**Reliability:** (4) not assignable
Secondary reference.
11-NOV-2004 (29)

**Remark:** A summary report of a rabbit eye irritation test carried out to OECD 405 on Nacol 6 RD for Condea Chimie GmbH in 1986. The result is given as moderately irritating with an EC classification of irritating. No further details are available.
**Test substance:** Tradename Nacol 6 RD
**Reliability:** (4) not assignable
Secondary reference.
11-NOV-2004 (29)

**Remark:** Data cited in Iuclid 2000.
**Test substance:** Reported as hexanol 98%
**Reliability:** (4) not assignable
17-OCT-2004 (21) (29)

## 5.3 Sensitization

**Type:** other: modified Draize test
**Species:** other: inbred Hartley albino guinea pigs
**Concentration 1st:** Induction .25 % intracutaneous
**2nd:** Challenge 10 % open epicutaneous
**3rd:** Challenge .1 % intracutaneous
**No. of Animals:** 10
**Vehicle:** no data
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other
**Year:** 1978

**GLP:** no data
**Test substance:** other TS: hexanol (random sample from commercial batch)

**Result:** RESULTS OF PILOT STUDY: 0.25%, 0.1% and 10% solutions were chosen for the intradermal induction, intradermal challenge and topical challenge respectively.
RESULTS OF TEST
- Sensitization reaction: No sensitisation reactions at challenge or rechallenge following a second induction procedure. The result was reported as non-sensitising, individual animal data were not presented.
- Clinical signs: None
- Rechallenge: No sensitisation

**Source:** Sharp 1978
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMAL Guinea pig
- Strain: Hartley
- Sex: not reported
- Source: not reported
- Weight at study initiation: ca 350 g
- Number of animals: 10
- Controls: only at rechallenge

ADMINISTRATION/EXPOSURE
- Study type: Non-adjuvant
- Preparation of test substance for induction: not reported, 0.1 ml of the test solution was administered.
- Induction schedule: 4 intradermal injections at one time point over the 2 auxillary and 2 inguinal lymph nodes.
- Concentrations used for induction: Based on a primary irritation screen the concentration used was 2.5 times the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema).
- Challenge schedule: 14 days after induction each animal received an intradermal injection in one flank and a topical application on the other.
- Concentrations used for challenge: 0.1% intradermally ad 10% topically
- Rechallenge: Where materials test negative at challenge a repeat set of induction applications was carried out followed by challenge at 14 days and rechallenge (with controls) 7 days later.
- Positive control: not reported

EXAMINATIONS
- Grading system: A colour matching lighting unit was used to examine the skin reactions. Each injection reaction was scored based on size, erythema and oedema and considered positive if the total score was greater than the total average of the control scores. Application reactions were scored on a scale of 0 to +++ and considered positive if individual reactions were => + and there was no erythema in the controls.

- Pilot study: A preliminary irritation study was undertaken to determine the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema) and the application challenge concentration (the highest concentration producing no irritation).

**Conclusion:** In this non-adjuvant procedure (modified Draize) hexanol was not a skin sensitiser in guinea pigs following intradermal and

topical challenge after 2 series of induction applications.
**Reliability:** (2) valid with restrictions
Reasonable reporting of a modified Draize test, result reporting limited. Test sample not fully characterised. Controls only included at rechallenge.
**Flag:** Critical study for SIDS endpoint
28-DEC-2005 (64)

**Type:** Patch-Test
**Species:** human

**Method:** other: human patch test
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These secondary references report that in a human patch test 1-hexanol (1% in petrolatum) was not a skin irritant or sensitiser.
**Reliability:** (4) not assignable
Secondary literature.
12-SEP-2004 (29) (46) (48)

**Remark:** Report of an M&K guinea pig maximisation test carried out by Henkel (report TBD 790129 also reported in Henkel report TBD900320). The test substance as prescribed was not a skin sensitiser.
**Test substance:** 1-hexanol
**Reliability:** (4) not assignable
Secondary reference
13-OCT-2004 (29)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** other: Albino rats **Sex:** male/female
**Strain:** other: ex Charles River
**Route of administration:** oral feed
**Exposure period:** 13 weeks
**Frequency of treatment:** daily
**Post exposure period:** none
**Doses:** 0.25% & 0.50% for 13 weeks; 1.0% for 10 weeks then 2.0% (week 11), 4.0% (week 12) and 6.0% (week 13).
**Control Group:** yes, concurrent no treatment
**NOAEL:** = 1127 mg/kg bw

**Method:** other: (see text)
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).
**Result:** NOAEL (NOEL): M 1127 mg/kg/day F 1243 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.25% M 182 mg/kg/day; F 216 mg/kg/day

0.5% M 374 mg/kg/day; F 427 mg/kg/day
1% M 1127 mg/kg/day; F 1243 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: One male at the lowest dose level (0.25%) died in the 9th week of the study. This was not attributed to treatment.
- Clinical signs: all surviving animals appeared normal.
- Body weight: comparable to controls.
- Food consumption: with the exception of high dose females at week 13 food consumption was comparable with that of controls. At week 13 female food consumption was 87.8% of control females at this time period. At this stage of the study the top dose level had been increased incrementally from 1% at week 10 to 6% in the diet at week 13.
- Clinical chemistry: not carried out.
- Haematology: No treatment related changes.
- Urinalysis: No treatment related changes.
- Organ weights: The original report indicates that there were significant differences in some relative organ weights from treated groups compared to controls. These were reanalysed by the Weinberg Group using the Tukey test which indicated that only the increased heart weight in mid dose males remained significant. The significant changes found in the original report together with the results of the Weinberg analysis are summarised below.

| Organ | Sex | Orig sig. | Weinberg report |
|---|---|---|---|
| Heart | M | mid-dose | Significant |
| Spleen | M | high dose | Not significant |
| | F | high dose | Not significant |
| | F | low dose | Not significant |
| Gonads | M | all levels | Not significant |

Additionally Weinberg reanalysed the organ weight data for the liver, kidney, adrenal, brain and thyroid none of which showed significant changes in the original statistical analysis. There were no significant changes except in the thyroid weight which showed a significant increase in top dose males according to the Weinberg analysis.

Statistical results are not reported in detail, while individual animal data are reported means are not given. Using this data to calculate the mean and SD for the organ weight changes originally reported as significant (see table above) the magnitude of the changes is a follows:

Spleen weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 0.185 | 0.175 | 0.19 | 0.199* |
| SD | 0.044 | 0.008 | 0.028 | 0.047 |
| Females | 0.189 | 0.223* | 0.189 | 0.217* |
| SD | 0.018 | 0.036 | 0.01 | 0.02 |

Gonad weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 0.793 | 0.809* | 0.814* | 0.804* |
| SD | 0.062 | 0.007 | 0.079 | 0.075 |

Heart weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 0.296 | 0.268 | 0.331*+ | 0.328 |
| SD | 0.005 | 0.002 | 0.074 | 0.041 |

*Significant using Chi square test as reported in original report. +Significant in Tukey test.

- Gross pathology: Unremarkable
- Histopathology: There were no treatment related histopathological changes in the control and top dose animals examined.

STATISTICAL RESULTS: Original organ weight analyses using the Chi square test were supplemented by Tukey tests carried out by the Weinberg group.

**Source:** Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: Actual age not reported, described as young.
- Weight at study initiation: M 103.8 g; F 90.4 g
- Number of animals: 10M + 10F per test group, 20M + 20 F controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 13 weeks
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 0.2, 0.5 and 1% in the diet. The 1% dose ws increased to 2% in week 11, 4% in week 12 and 6% in week 13.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily (5 days/week)
- Mortality: Daily (5 days/week)
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: Not carried out.
- Haematology: At 30 days and 90 days on 5M+5F. Micro haematocrit, Hb, total & differential leucocytes.
- Biochemistry: Not carried out.
- Urinalysis: At 30 days and 90 days on pooled samples from 5 rats of each sex.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Complete necropsy performed, organ weights measured were brain, thyroid, heart, liver, spleen, kidneys, adreanls and gonads.
- Microscopic: Tissues fixed: brain, thyroid, parathyroid, heart, lung, liver, spleen, stomach, small & large intestine, pancreas, kidney, urinary bladder, adrenals, gonads, lymph node, bone, bone marrow, muscle. All tissues from 5M+5F high dose and control animals were examined.

STATISTICAL METHODS: The original report indicates that a Chi square test was carried out on the organ:bodyweight ratio. It is not clear what statistical methods were used (if they were) for body weights, food consumption & haematological parameters. Subsequently The Weinberg Group Inc. used Tukeys

test to re-analyse the organ weight data.
**Test substance:** Tradename is Alfol 6. Sample supplied by the Continental Oil Co. Louisiana (1965).
**Conclusion:** The NOAEL for Alfol 6 in rats following 13 week dietary exposure is 1127 mg/kg for males and 1243 mg/kg (highest test doses) for females (highest test doses) based on a lack of toxicologically significant effects at any dose level. The significant increase in relative heart weight in mid-dose males was not dose related and not correlated with histopathological change and was therefore not considered biologically significant. This was the only organ weight effect which was significant using both Chi square and Tukeys test. There were no histopathological changes in any organ.

Reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment of the limited parameters assessed.
**Flag:** Critical study for SIDS endpoint
02-JAN-2006 (29) (60)

**Type:** Sub-chronic
**Species:** dog **Sex:** male/female
**Strain:** Beagle
**Route of administration:** other: dietary at 0.5 & 1% (low & mid dose), high dose 1000 mg/kg/day by capsule
**Exposure period:** 13 weeks
**Frequency of treatment:** daily for dietary administration, 6 days/week via capsules.
**Post exposure period:** none
**Doses:** 0.5, 1.0% w/w and 1000 mg/kg/day
**Control Group:** yes, concurrent no treatment
**NOAEL:** = 370 - 435 mg/kg bw
**LOAEL:** = 1000 mg/kg bw

**Method:** other: see test conditions
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).
**Result:** NOAEL (NOEL), LOAEL (LOEL): M 370 mg/kg/day; F 435 mg/kg/day (M+F 403 mg/kg/day); LOEL 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.5% M 199 F 190 mg/kg/day
1% M 370 F 435 mg/kg/day
Top dose 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: 1000 mg/kg both males died day 23 & 38. Both females died day 1 & day 38. Another female was included which survived the 13 week exposure period. All control, lower & mid dose animals survived the exposure period.

- Clinical signs: 1000 mg/kd/day signs seen in all dogs, at some stage during the dosing period, were salivation, emesis,

mild excitation, ataxia, slight tremors and varying stages of anaesthesia (which preceded death in all animals which died). No specific clinical signs in lower dose or control animals.

- Body weight gain: No difference from control values for the low & mid dose groups.

- Food consumption: No difference from control values for the low & mid dose groups.

- Ophthalmoscopic examination: Not done
- Clinical chemistry, Haematology, Urinalysis: No apparent differences between treated and control groups.

- Organ weights: No difference from control values for the low & mid dose groups.

- Gross pathology: Lymph node hyperplasia in both control & treated animals considered due to roundworm infestation (despite routine deworming throughout the study). In all animals which died there was evidence that the dogs may have aspirated vomit while anaesthetised (as a result of exposure to Alfol 6), death resulting from respiratory crisis. There was evidence of food particles in the trachea and the respiratory system smelled of the test substance.

- Histopathology: In top dose (1000 mg/kg/day) animals and to a lesser extent in animals of the intermediate dose level there was evidence of gastro-intestinal irritation (mucosal hyperemia without ulceration or acute inflammatory reaction). The 2 high dose males (both died) showed testicular atrophy while one high dose female which died showed decreased oogenesis, the ovaries of the female which surived exposure to the high dose level appeared within normal limits. Other than gastro-intestinal irritation in mid dose animals there were no other treatment related hisptopathological changes in dogs receiving 0.5 or 1% Alfol 6 in the diet.

- Other: ECG's showed no differences between the initial pattern recorded and those seen at 3 or 13 weeks.

STATISTICAL RESULTS: Analysis not carried out. Subsequent analysis of the data using Tukeys Test indicates no significant differences in organ weight data.

**Source:** Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 5 months
- Weight at study initiation: M4.77-8.97 kg; F4.31-7.95 kg
- Number of animals: 2M+2F treated; 4M+5F controls

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 13 weeks
- Type of exposure: 0.5% and 1% in the diet (low and mid dose) daily, 1000 mg/kg/day as a gelatin capsule 6 days/week (high dose, dietary high dose was unpalatable).
- Post exposure period: None
- Vehicle: Diet, none for top dose level(gelatin capsule).
- Doses: 0.5 and 1% in diet, 1000 mg/kg by gelatin capsules.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily 5 days/week. Complete physical examination, body temperature, pulse rate, reflexes, mucous membranes, auscultation pretreatment, 3, 6 & 13 weeks. ECG pretreatment, 3 and 13 weeks.
- Mortality: Daily (5 days/week?)
- Body weight: weekly
- Food consumption: weekly
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Not recorded.
- Haematology: Total & differential leucocyte counts, Hb, haematocrit, erythrocyte sedimentation rate, prothrombin time measured pretreatment, 3, 6 and 13 weeks.
- Biochemistry: Plasma levels of glucose, total protein & albumin, albumin/globulin ratios, urea nitrogen measured pretreatment, 3, 6 and 13 weeks. Liver function assessed by BSP retention, alkaline phosphatase & ASAT at same time periods.
- Urinalysis: albumin, glucose, bilirubin, pH, vol. , specific gravity, microscopic examination of sediment, total nitrogen. Carried out pretreatemnt & at 3, 6 & 13 weeks.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: complete, organ weights determined for brain, thyroid, heart, liver, kidneys, adrenals, spleen, gonads.
- Microscopic: Brain, pituitary, sub-maxillary salivary gland, thyroid, parathyroid, heart, lung, liver, spleen, stomach (fundic & pyloric), small intestine (3 levels), large intestine, pancreas, gall bladder, kidney, urinary bladder, adrenal, gonads, lymph node (cervical & mesenteric), bone, bone marrow, muscle (striated). All fixed. Tissues from controls & high dose animals examined microscopically. Stomach & intestinal tissues from mid dose animals also examined plus any abnormal tissues identified at necropsy.

STATISTICAL METHODS: No statistical analysis reported in the original report. For the HPV program the results were analysed using Tukey's Test.

**Test substance:** Tradename Alfol 6.

**Conclusion:** The NOAEL for Alfol 6 is considered to be 370 mg/kg day for male dogs and 435 mg/kg/day for females (dietary administration). The treshold for irritation of the gastrointestinal tract was 190 mg/kg/day. High dose animals showed evidence of testicular atrophy 2/2 or decreased oogenesis 1/2. These animals died during the study and the effects are attributed to the acute lethality of the test substance adminstered at 1000 mg/kg by capsule. There were no adverse effects on the gonads at the lower dose levels. The value of this study is limited by the small numbers of test animals and the toxicity of the high dose level.

Reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
This study has methodological deficiences, animal group size too small (only 2M+2F in test groups), no statistical analysis, high mortality in top dose level which was administered by capsule while lower dose levels were administered in the diet. Useful as supporting data.

**Flag:** Critical study for SIDS endpoint

09-JAN-2006 (29) (61)

**Type:** Sub-acute
**Species:** rat **Sex:** male
**Strain:** Fischer 344
**Route of administration:** oral feed
**Exposure period:** 3 weeks
**Frequency of treatment:** continuous
**Post exposure period:** none
**Doses:** 2, 4 and 8%
**Control Group:** yes
**NOAEL:** > 8 %

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** 1-hexanol did not have any significant effect on relative liver to body weight, liver catalase, liver carnitine acetyl transferase or hepatic peroxisome proliferation or in serum lipids compared to the control group. Results were presented for the 2% dietary level but the authors indicate that 1-hexanol was also tested at dose levels or 4 and 8% with no adverse effects. 2-ethyl hexyl alcohol at 2% produced statistically significant ($p<0.001$) increases in all the above parameters except body weight and a decrease in serum triglycerides and cholesterol. The results of the serum lipid determinations are reported in a later publication (Moody & Reddy, 1982)

**Test condition:** The purpose of this study was to investigate the effects of various plasiticisers including DEHP and related materials on hepatic peroxisome proliferation and associated changes in liver parameters. 1-hexanol was included for comparison.

A group of 5 male rats received 2% 1-hexanol in the diet for 3 weeks, an untreated group of 13 male rats served as controls. The rats, housed individually, weighed 150-180 grams at the start of the study.

At the end of the exposure period the rats were sacrificed and blood, drawn from the abdominal aorta, was used for measurement of serum cholesterol and triglycerides. Liver sections were taken for electron microscopy. Liver carnitine acetyl transferase and hepatic catalase were measured spectrophotometrically.

Statistically evaluation was made using the students t-test.

Results are presented for the dietary level of 2% however the authors indicate that 1-hexanol was tested at 4 and 8% (results not reported).

**Conclusion:** Administration of up to 8% 1-hexanol in the diet of male rats for a period of 3 weeks did not in increase peroxisome proliferation or affect serum triglycerides or cholesterol. Reported in Patty, 2001.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

15-JUL-2005 (38) (39) (48)

**Type:** Sub-chronic
**Species:** rabbit **Sex:**
**Route of administration:** inhalation
**Exposure period:** 6 months
**Frequency of treatment:** not reported
**Doses:** 28.3 ppm
**Control Group:** no data specified

**Method:** other: no data
**Year:** 1971
**GLP:** no
**Test substance:** other TS: described as hexanol but not specifically identified as 1-hexanol

**Remark:** Limited reporting of a 1971 Russian study in which electron microscopic examination of the retina of the eyes of rabbits exposed by inhalation to vapours of 118 mg/m3 (28.3 ppm) hexyl alcohol for 6 months revealed ultrastructural changes in the photoreceptor cells and Muller fibres. No further experimental details were available. While referred to in Patty 2001, the fuller report is to be found in Patty 1982. This study also appears to be reported in RTECS.
**Reliability:** (4) not assignable
Secondary literature. original reference in Russian and unobtainable.
13-OCT-2004 (47) (48) (55)

**Type:** Sub-chronic
**Species:** rat **Sex:**
**Strain:** Sprague-Dawley
**Route of administration:** i.p.
**Exposure period:** 30 weeks
**Frequency of treatment:** Daily, 6 days/week
**Post exposure period:** None
**Doses:** 102.5 mg/kg/day
**Control Group:** yes, concurrent vehicle

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** This study was carried out to investigate the possible peripheral neurotoxicity of 1-hexanol (and 2-hexanol) known metabolites of the known peripheral neurotoxin n-hexane.

1-hexanol did not produce the typical EMG alterations observed with n-hexane and in particular the distal motor latency was unchanged. There were also no clear cut abnormalities of the peripheral nerve. The relevance of the decrease in sensory conduction velocity is unclear.
**Test condition:** Groups of male rats (10 controls, 20 treated) weighing 340-350 g, received a single ip dose of 1-hexanol (12.5% in peanut oil) daily 6, days/week for 30 weeks. Controls received the same volume of peanut oil (1 ml/kg) as the treated group.

The rats were examined clinically weekly. At 8 weeks and again at the end of the test period the rats were subjected to

neurophysiological examinations (electromyograph).

Measurements were made of motor and sensory conduction velocity, sensory potential amplitude and distal motor latency.

After the neurophysiological examinations at the end of the study 2 rats from each group were sacrificed and the peripheral nerves were removed and examined after suitable treatment.

Dunnetts test was used to assess statistical significance.

**Test substance:** 1-hexanol >98% pure

**Conclusion:** This neurophysiological investigation in rats following long term exposure to 1-hexanol indicates that 1-hexanol (n-hexane metabolite) does not produce the the typical changes in EMG characteristic of peripheral neuropathy induced by n-hexane.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

29-SEP-2004 (49)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames Test)
**System of testing:** Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
**Concentration:** 1st test: 8,40, 200, 1000 and 5000 ug/plate 2nd test: 6.25, 25, 100, 400 and 1600 ug/plate
**Cytotoxic Concentration:** 5000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1990
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No significant increase above control levels in either series of tests.

PRECIPITATION CONCENTRATION: No precipitation.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: complete or partial inhibition of background lawn observed in all strains at 5000 ug/plate (except TA 100 where no inhibiton was observed)

TEST-SPECIFIC CONFOUNDING FACTORS: None

**Source:** Henkel 1990
Hayes Consultancy Service Bromley, Kent

**Test condition:** METHOD
Bacterial reverse mutation assay OECD 471. 2-aminoanthracene was the only indicator of S9 efficacy, however all the cultures treated with 2-AA in the presence of S9, showed a clear increase in reverse mutation rate compared to controls. The activity of the S9 was confirmed against strain TA98 using 2AA and benzo[a]pyrene. A cytogenetic test with

cyclophosphamide was also carried out.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium stains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced. The activity of the S9 was confirmed against strain TA98 using 2AA and benzo[a]pyrene. A cytogenetic test with cyclophosphamide was also carried out.

ADMINISTRATION:
- Dosing: 1st test: 8,40, 200, 1000 and 5000 ug/plate
2nd test: 6.25, 25, 100, 400 and 1600 ug/plate suspended in Tween 80/aqueous.
- Number of replicates: three
- Application: Plate incorporation
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate all strains; sodium azide 2 ug/plate; 9-amino acridine (80 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate. Negative controls Tween 80/aqueous and untreated fresh cell suspensions in buffer.
- Incubation: 48 hours at 37C

CRITERIA FOR EVALUATING RESULTS: Combination of: a) Plate background of non-reverted bacteria not showing growth reduction vs respective negative controls. b) Spontaneous mutation rates within historical limits. c) At one or more doses tested the substance causes a 2 (TA 100) or 3 (other strains) fold increase in mutation rate above control levels.

**Test substance:** Tradename Lorol C6 (98% pure)

**Conclusion:** The C6 alcohol Lorol C6 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate (cytotoxicity observed at 5000 ug/plate).

Reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

11-NOV-2004 (25) (29)

## 5.6 Genetic Toxicity 'in Vivo'

**Type:** Sister chromatid exchange assay
**Species:** Chinese hamster **Sex:** no data
**Route of admin.:** i.p.

**Method:** other: In vivo sister chromatid exchange
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no increase in sister chromatid exchange in the cells treated with 1-hexanol alone 2.9 +-0.3 SCE/cell), the level of SCE was comparable with controls (2.9 +-0.1 SCE/cell). When injected in the presence of NMU 1-hexanol

reduced the incidence of SCE compare to NMU given alone.

**Test condition:** 1-hexanol prepared as an emulsion in saline was injected intraperitoneally into a single Chinese hamster aged between 12-13 weeks of age and weighing ca 30g at a dose level of 10(-3) moles/kg bw. 2 control animals received an injection of water. All animals received a subcutaneous implant of BrdU in the neck prior to treatment and injection of colchicine 2 hours before sacrifice at 24 hours. 50 cells from the control animals and 25 from the treated animal were scored for induction of SCE. The study was carried out as part of an investigation of the effects of n-alkanols on the induction of SCE by NMU and NMU acted as a positive control.

**Reliability:** (3) invalid
Significant methodological deficiencies, use of only one test animal limits the validity of this study. In the secondary publication by Tucker et al, 1993 this study is considered as inadequate or equivocal.

12-SEP-2005 (69) (71)

**Type:** Cytogenetic assay
**Species:** rat **Sex:** male
**Strain:** other: unspecified
**Route of admin.:** other: intragastric
**Exposure period:** 48 hours
**Doses:** 1/5th LD50
**Result:** ambiguous

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:

600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 2.8 +-0.7
Cells with breakages %: controls 0.3 +-0.2; treated 0.4 +-0.2;
Cells with chromosome aberrations %: controls 0; treated 2.8 +-0.7.

STATISTICAL RESULTS: Reported as above.

**Source:** Barilyak, 1988
**Test condition:** TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage

- Vehicle: Homogenised emulsion
- Duration of test: 48 hours
- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Conclusion:** Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability:** (3) invalid
Significant methodological deficiences (see test conditions).

08-OCT-2004 (8)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** In common with other members of the aliphatic alcohols category 1-hexanol contains no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the range of category members including 1-hexanol are negative. Results from in vivo studies with other category members and/or supporting substances provide evidence that these alcohols are not genotoxic in vivo.

Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline studies or publications with sufficient detail for assessment.
12-SEP-2005 (28) (66) (67) (74)

## 5.7 Carcinogenicity

**Species:** mouse **Sex:** female
**Strain:** Swiss
**Route of administration:** dermal
**Exposure period:** 60 weeks
**Frequency of treatment:** three times weekly
**Post exposure period:** none
**Doses:** 4 ug/mouse in cyclohexane
**Result:** negative
**Control Group:** no

**Method:** other: skin tumour promotion study
**Year:** 1966
**GLP:** no data
**Test substance:** other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.
**Source:** Sice 1966.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group
ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane
- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)

- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Test substance:** The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Conclusion:** In this comparative study, published in 1966, the authors investigated the tumour promoting activity of C6-C18 alkanols. Hexanol was inactive in this test system.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

12-SEP-2004 (29) (45) (48) (65)

## 5.8.1 Toxicity to Fertility

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** rat
**Sex:** male/female
**Strain:** other: Charles River
**Route of administration:** oral feed
**Exposure Period:** 13 weeks
**Frequency of treatment:** daily
**Duration of test:** 13 weeks
**Doses:** 0.25, 0.50, 1.0, 2.0, 4.0, and 6.0% w/w
**Control Group:** yes
**NOAEL Parental:** = 1127 - 1243 mg/kg bw

**Method:** other
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).

**Result:** None of the animals displayed gross effects of oral exposure to hexanol during the 13-weeks of the experiment. Food consumption and body weights were comparable to the controls. No haematological changes were evident in any animals. Terminal organ weights (heart, spleen, gonads) were sporadically different from controls at different times. The original study report indicated significant differences between control and treated testes weights at all dose levels. No indication was given of which statistical method was used to analyse the data. Weinberg Associates reanalysed the data using a Tukey test and found that male gonad weights were not significantly different from the controls at any test concentration. There were no histopathological changes in any

organs examined including the gonads. The NOAEL for reproductive endpoints is therefore the highest dose level (1243 mg/kg bw for females and 1127 mg/kg/day for males).

**Source:** Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 20 rats (10 of each sex) were fed hexanol in the diet for 13 weeks. The control group consisted of 20 males and 20 females. The doses used were 0.25% w/w, low dose, 0.50% w/w, intermediate dose, and 1.00% w/w, high dose for weeks 1-10. They were fed 2.00% w/w for week 11, 4.00% w/w for week 12 and 6.00% w/w for week 13. At termination, all animals were sacrificed, necropsied, and tissues from 5 males and 5 females from the control and top dose groups were examined histopathologically. Fuller study details are reported in Chapter 5.4 Repeated dose toxicity.

**Test substance:** Tradename Alfol 6.

**Conclusion:** NOAEL for reproductive endpoints, 1243 mg/kg/day in females, 1127 mg/kg/day for males based on organ weights and histopathology of the gonads which showed no significant changes.

**Reliability:** (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

07-SEP-2004 (60)

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** dog
**Sex:** male/female
**Strain:** Beagle
**Route of administration:** oral feed
**Exposure Period:** 13 weeks
**Frequency of treatment:** daily
**Duration of test:** 13 weeks
**Doses:** 0.5, 1.0% w/w and 1000 mg/kg/day
**Control Group:** yes
**NOAEL Parental:** = 370 mg/kg bw

**Method:** other
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).

**Result:** In the highest level (~1100 mg/kg/day), all of the animals displayed signs of toxicity which consisted of salivation, excitation, ataxia, tremors, and anaesthesia and resulted in the death of both males and 2/3 females. There was also evidence of gastrointestinal inflammation and gonadal atrophy. Histopathological examination revealed testicular atrophy in the males which died and decreased oogenesis in one female. The ovaries of the surviving top dose female appeared normal. The gonadal changes were attributed to general ill health rather than direct toxic effects.

There were no adverse effects on the histopathology of the

ovary or testes at the lower dose levels tested and no apparent effect on the organ weights. The value of this study is limited by the small numbers of animals used.

The NOAEL for reproductive endpoints was 370 mg/kg/day.

**Source:** Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 4 Beagle dogs (2 of each sex) were exposed to 0.5, 1.0% w/w in the diet and 1000 mg/kg/day via gelatin capsule for 13 weeks. The control group contained 4 males and 4 females. At termination, all animals were sacrificed and necropsied. Full details of this study are reported in Chapter 5.4 Repeat dose toxicity.

**Test substance:** Tradename Alfol 6.

**Conclusion:** NOAEL 370 mg/kg/day (dietary administration of 1% test compound) for reproductive effects based on lack of histopathology in the gonads and no effect on reproductive organ weights. This was also the NOAEL for general systemic effects.

**Reliability:** (2) valid with restrictions
This study has methodological deficiences, animal group size too small (only 2M+2F in test groups), no statistical analysis, high mortality in top dose level which was administered by capsule while lower dose levels were administered in the diet. Useful as supporting data.

13-OCT-2004 (61)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Species:** rat **Sex:** female
**Strain:** Sprague-Dawley
**Route of administration:** inhalation
**Exposure period:** days 1-19 of gestation
**Frequency of treatment:** 7 hours/day
**Duration of test:** 20 days
**Doses:** 3500 mg/m3
**Control Group:** yes
**NOAEL Maternal Toxity:** = 3.5 mg/l
**NOAEL Teratogenicity:** = 3.5 mg/l

**Method:** other: see text
**Year:** 1989
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL : 3.5 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5% of the nominal concentration of 3.5 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: There was a significant increase in

mean resorption/litter (p<0.05). 1-hexanol treated 1.3, controls 0.4. This was within the historical control range which is reported as up to 1.3 resorptions per litter. The actual control value was at the lower end of the range of values found among 11 control groups used in a series of similar studies by these authors over a 5 year period (Nelson et al 1990b). The range of resorptions in these control groups was 0.2 -1.5 per litter (mean 0.9) further suggesting that this was not a treatment related effect.
- Number of implantations: Values not given although as numbers were recorded assume there was no difference between treated and controls.
- Number of corpora lutea: Comparable between treated and control groups. Corpora lutea/litter controls 17 +- 1, treated 14 +- 4.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Food consumption significantly higher than controls (p<0.05); water consumption unaffected.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Mean foetal weight treated - males 3.19 g, females 3.05g; controls - males 3.28 g, females 3.19 g. Litter size (mean) treated and control 15.
- Sex ratio: No significant difference between treated and controls. Sex ratio - controls 7F, 8M; Treated 8F,7M.
- Grossly visible abnormalities: None
- External abnormalities: None
- Soft tissue abnormalities: None
- Skeletal abnormalities: There were small insignificant delays in ossification of caudal vertebrae, sternum, metacarpals and hind paw phalanges indicative of growth retardation but which were not accompanied by effects on foetal weight. Data not presented.

**Source:** Nelson, et al. 1989.
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
Groups of approximately 15 female rats weighing 200-300g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose: 3.5 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F.

MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC): Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA

**Conclusion:** The NOAEL for maternal toxicity, foetotoxicity and teratogencity in rats, following inhalation exposure to n-hexanol on gestation days 1-19, is 3.5 mg/l (850 ppm), the highest atmospheric concentration which could be generated. There was no maternal toxicity based on clinical observations and bodyweight measurement. Reproductive indices were unaffected by treatment. An apparent increase in the number of resorptions was within historical control limits and within the limits of a series of control groups from comparable studies. Combined with the particularly low incidence of resorptions in the control groups this observation is not considered treatment related.

Reported in Iuclid 2000 and Patty 2001.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (29) (43) (44) (48)

**Species:** rat **Sex:** female
**Strain:** other: COBS CD
**Route of administration:** gavage
**Exposure period:** days 6-15 of gestation
**Frequency of treatment:** daily
**Duration of test:** through day 20 of gestation
**Doses:** 200 and 1000 mg/kg bw
**Control Group:** yes
**NOAEL Maternal Toxity:** = 200 mg/kg bw
**NOAEL Teratogenicity:** = 1000 mg/kg bw

**Method:** other: see text
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Maternal toxicity at 1000 mg/kg/day was evidenced by reduced body weight and clinical signs of intoxication. No further details are available. There were no signs of maternal toxicity at 200 mg/kg/day.

There was no evidence of teratogenicity in this study. Effects on the foetus were confined to an increase in numbers of litters with the skeletal variant 'malaligned sternebrae' which occured at 200 mg/kg/day only and a slight decrease in foetal weight at 1000 mg/kg/day which was within the historical control range.

As an increased incidence of 'malaligned sternebrae' was not observed at 1000 mg/kg/day the observation at 200 mg/kg/day was considered incidental.

**Source:** Rodwell 1988.
Hayes Consultancy Service Bromley, Kent

**Test condition:** Summary data only are available for this study. Groups of 25 bred female COBS CD rats received either 200 or 1000 mg/kg/day 1-hexanol daily by gavage on gestation days 6-15. the test material was administered in corn oil at a volume 5 ml/kg, a vehicle control group was included. Appearance, behaviour and body weights were recorded throughout the gestation. The dams were sacrificed and sectioned on gestation day 20. Intrauterine survival, foetal weight and external, skeletal and visceral anomalies were recorded.

**Conclusion:** The NOAEL for maternal toxicity in rats, following exposure by gavage to n-hexanol on gestation days 6-15, is considered to be 200 mg/kg/day based on clinical signs of toxicity and reduction in bodyweight at the higher dose level of 1000 mg/kg/day. The NOAEL for teratogenicity and foetotoxicity is considered to be 1000 mg/kg/day based on absence of adverse effects at this dose level (highest tested). A slight decrease in foetal weights was within historical control limits.

Reported in Patty 2001.

**Reliability:** (4) not assignable
Abstract only available.

11-NOV-2004 (48) (54)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: human skin irritation

**Result:** In this inter-laboratory assessment of the human patch test hexanol gave responses significantly lower than the positive control and results were similar between laboratories. N-hexanol was therefore not considered as a skin irritant.

**Source:** Griffiths et al, 1997
Hayes Consultancy Service Bromley, Kent

**Test condition:** These materials were tested as part of an interlaboratory evaluation of a human patch test for identification of skin irritation potential.

Groups of at least 30 volunteers were used for each evaluation at each location, at least 2 locations tested each product. The undiluted material (0.2 ml) was applied to the outer arm using a Hill Top chamber for a period usually of 4 hours. The reaction was assessed at 24, 48 and 72 hours after initiation of the exposure. SDS (sodium dodecyl sulphate) was used as a positive control. If the proportion of the test group reacting to the test material was significantly less that those reacting to the positive control the material was considered as not classifiable as a skin irritant.

**Test substance:** hexanol, octanol, decanol

**Reliability:** (2) valid with restrictions
Study well-documented, meeting generally accepted scientific principles, acceptable for assessment.

29-SEP-2004 (23)

**Type:** other: aspiration

**Remark:** Aspiration of 0.2 ml 1-hexanol to rats produced immediate death in 10/10 rats following respiratory arrest.

**Test substance:** 1-hexanol

**Reliability:** (2) valid with restrictions

29-SEP-2004 (22) (48) (48)

**Type:** other: sensory irritation

**Remark:** The RD50 for n-hexanol was reported as 240 ppm in Swiss mice. Exposure time not reported. The original paper (Muller & Greff, 1984) reports unpublished data which is summarised in Bos et al, 1992.

**Test substance:** 1-hexanol

**Reliability:** (4) not assignable
Secondary report

29-SEP-2004 (10) (41)

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

(6) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(7) Associates, Inc. 1977c. Acute oral toxicity (LD50) in rats; Acute dermal toxicity (LD50) in rabbits, Dermal irritation test in rabbits; Eye irritation test in rabbits; Inhalation toxicity tests in rats: ALFOL 6. S.A. Number 233619.

(8) Barilyak, I.R.; Kozachnuk, S.Yu. 1988 Investigation of the cytogenetic effect of a range of monohydric alcohols on bone-marrow cells of rats. Tsitologiya i Genetika 22(2):49-52 (Russian language, translation available)

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 111-87-5 |
| **CAS No.** | 111-87-5 |
| **EINECS Name** | octan-1-ol |
| **EC No.** | 203-917-6 |
| **TSCA Name** | 1-Octanol |
| **Molecular Formula** | C8H18O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **116** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK, The Environment Agency
**Contact Person:** Steve Dungey **Date:**
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**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

28-SEP-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium Member
19-SEP-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
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**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Scott Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Members
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc
**Contact Person:** Dave Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston,TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Olefins and Surfactants GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** Paul-Baumann-Strasse, 1
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77210 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
02-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |

| | |
|---|---|
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

02-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Octanol
**Smiles Code:** OCCCCCCCC
**Mol. Formula:** C8 H18 O1
**Mol. Weight:** 130.23

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-octanol, CAS 111-87-5 are 100% linear.

The substance comprises >90% C8. Components of even chain length, in the range C6-C10 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:
1-Octanol (9CI) (CA INDEX NAME)
Octyl alcohol (8CI)
Lorol C 8-98
n-Octan-1-ol
n-Octanol
n-Octyl alcohol
NSC 9823
Octanol
Octilin
Sipol L8
Octan-1-ol
1-octyl alcohol
Alcohol C-8
n-Caprylic Alcohol
Capryl alcohol
n-Capryl Alcohol

Some commercial products with the name CO
1-Hydroxyoctane
Alfol 8
Caprylic alcohol
CO 898
CO 898 (solvent)
Heptyl carbinol
Kalcohl 0898
Alfol 8 Alcohol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-octanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey

of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >25 000 - 50 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >50 000 000 - 100 000 000 pounds.

Japan: Consumption 3000 tonnes (CAS-specific data)- This is publicly-available CEH data for Japan, for 2001.

21-DEC-2005 (7) (81) (115)

### 1.6.1 Labelling

**Remark:** Not required

11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required

11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

**-**

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 50 Surface-active agents

**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 50 Surface-active agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 2 Adhesive, binding agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 38 Plant protection products, agricultural
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents

typical composition. Specific batches may be subject to variation.
21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 165.
05-AUG-2005 (124)

## 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

## 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

**CAS-No:** 111-87-5
**EC-No:** 203-917-6
**EINECS-Name:** octan-1-ol

05-AUG-2005

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-octanol. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

02-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

02-AUG-2005

## 2.1 Melting Point

**Value:** = -15.5 - -17 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (31)

**Value:** = -18 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (95)

**Value:** = -16.7 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (97)

**Value:** = -16.3 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment
03-JAN-2005 (78)

## 2.2 Boiling Point

**Value:** = 194 - 195 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (31)

**Value:** = 185 - 210 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (95)

**Value:** = 194.5 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (97)

## 2.3 Density

**Value:** = .826

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (118)

**Value:** = .82 - .83

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test conducted at 20 degrees C
**Reliability:** (4) not assignable
11-OCT-2005 (63)

**Type:** density
**Value:** = .815 - .825 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (95)

**Type:** density
**Value:** = .8254 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (40)

**Type:** density
**Value:** = .827 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (97)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .1 hPa at 25 degree C

**Method:** other (measured)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (37)

**Value:** = 1.3 hPa at 54 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (122)

**Value:** = .031 hPa at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (34)

**Value:** = 1.33 at 54 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (76)

**Value:** = 2.2 hPa at 60.1 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed secondary data source (Beilstein).
03-JAN-2005 (17)

**Value:** = 50.64 hPa at 113.3 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (21)

**Value:** .11 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis
**Reliability:** (2) valid with restrictions
Valid with restrictions.

The value was predicted using a partial vapour pressure contribution method, supported by additional validation
09-AUG-2005 (3)

## 2.5 Partition Coefficient

**log Pow:** = 3.15

**Method:** other (measured): No particulars on method stated.
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Several estimated values were presented in IUCLID 2000. The estimated values are of the same order as this measurement but are of lower reliability and are not presented here.
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for octanol-water partition coefficient values.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (45)

**log Pow:** = 2.8

**Method:** other (measured): No particulars on method stated.
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (73) (128)

**log Pow:** = 3.07

**Method:** other (measured): No particulars on method stated.
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. The original source is not stated.
03-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 551 mg/l

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Valid with restrictions. Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for solubility values.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (126)

**Solubility in:** Water
**Value:** = 495 - 596 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (122)

**Solubility in:** Water
**Value:** = 540 mg/l at 25 degree C

**Method:** other: measured
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** SRC.
**Reliability:** (4) not assignable
03-JAN-2005 (14)

**Value:** = 300 mg/l at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (122)

**Value:** = 495 mg/l at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (72)

**Value:** = 586.17 mg/l at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (18)

**Solubility in:** Water
**Value:** = 560 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 560 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
09-AUG-2005 (3)

**Solubility in:** Water
**Value:** = 500 mg/l at 25 degree C

**Method:** other: measured
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
This information was obtained from an authoritative, peer-reviewed secondary data source (Beilstein).
21-SEP-2005 (16)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 90 degree C
**Type:** closed cup

**Method:** other: DIN 51758
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
11-OCT-2005 (95)

**Value:** = 81 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature.
11-OCT-2005 (56)

**Value:** = 81 degree C
**Type:** other

**Method:** other: No information on method provided.
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning

this endpoint.
11-OCT-2005 (34)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (63)

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** no explosive properties are expected on the grounds of chemical structure
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** no oxidising properties are expected on the grounds of chemical structure
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Method:** other (measured): method not stated
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Measured rate constant: 14.4E-12 cm3/molecule.sec
Half-life: 26.7 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of atmospheric degradation data.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (11)

**Remark:** The photooxidation half-life in air for the gas-phase reaction with hydroxyl radicals was 0.24-2.4 hours, based on the rate of disappearance of hydrocarbon. The measured rate constant of 1.195x10-11 cm3/molecule*sec for the vapor-phase reaction with photochemically produced hydroxyl radicals of 5x10E5/cm3 at 25 C in air corresponds to an atmospheric half-life of 1.3 days.
**Reliability:** (2) valid with restrictions
29-DEC-2005 (9) (36)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The rate constant for the vapor-phase reaction of octanol with photochemically produced hydroxyl radicals in air has been estimated to be 1.195x10-11 cm3/molecule*sec at 25 C, which corresponds to an atmospheric half-life of about 1.3 days at an atmospheric concentration of 5x10E5 hydroxyl radicals/cm3.
**Test substance:** Octanol (111-87-5)
**Reliability:** (4) not assignable
Textbook used for background information.
29-DEC-2005 (10) (79) (107)

## 3.1.2 Stability in Water

**Type:** abiotic

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Photolysis or hydrolysis of octanol in aquatic systems is not expected to be important.
**Reliability:** (4) not assignable
Textbook used for background information.

**Flag:** Critical study for SIDS endpoint
10-JAN-2005 (79) (114)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Alcohols are generally resistant to hydrolysis. Alcohols absorb UV light at wavelengths <185 nm, which is not in the environmentally significant range of >290 nm. Likewise, alcohols are commonly used as solvents for obtaining UV spectra. Therefore octanol probably will not undergo hydrolysis or direct photolysis in the environment.
**Source:** Atkinson, R. 1987b. Intern. J. Chem. Kin. 19:799-828. (cited in HSDB)
**Test substance:** Octanol (111-87-5)
**Reliability:** (4) not assignable
Textbook used for background information.
11-OCT-2005 (10) (79) (107)

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Remark:** An evaporation rate of 1.75x10-6 mol/cm2*h was determined by gravimetric method with an air flow rate of 50 L/h at 20 C.Based on calculated Henry's law constant, half-life from a model river of 1 meter deep flowing at 1 m/sec with a wind speed of 3 m/sec has been estimated to be 1.8 days. The half-life from a model pond with the consideration of adsorption, has been estimated to be about 82 days.
**Result:** INPUT DATA USED:
Molecular weight 130.2
Data temperature 25 deg C
Log Kow 3.15
Water Solubility 551 mg/l
Vapour pressure 10 Pa
Melting point -16 deg C
half life in air 26.7 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:
Air 17.3%
Soil 45.4%

Water 36.3%
Fish 2.56E-03%
Sediment 1.01%

The Level III program has also been used, with the default model, using the same input parameters.
The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 63.6 | 0.0407 | 0.00446 |
| % in water | 4.02 | 98.7 | 1.6 |
| % in sediment | 0.0504 | 1.24 | 0.02 |
| % in soil | 32.3 | 0.0207 | 98.4 |

The results reflect that the ultimate fate of 1-octanol is dependent on its route of release into the environment. 1-Octanol released to air would partially precipitate to soil.There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.

**Test substance:** As prescribed in 1.1 - 1.4
**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 3.15 was used in the TGD calculation methods.

**Result:**
TGD Hydrophobics method: Koc = 448
TGD Non-hydrophobics method: Koc = 455.0
TGD Alcohols method: Koc = 53.5
SRC PCKOCWIN method: Koc = 28.3

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (5)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 92 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**
7 day(s) = 70 %
14 day(s) = 87 %
21 day(s) = 77 %
28 day(s) = 92 %
**Control Subst.:** Aniline

**Method:** other: ISO ring test "CO2 headspace biodegradation test"
**Year:** 1995
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were fulfilled
(1) the reference substance degraded by >60% after 14 days and

(2) the total inorganic carbon (TIC) present in the blank controls at the end of the test was less than 15% of the organic carbon added initially as the test substance. TIC at Day 0 was not reported.
**Result:** Kinetic of control substance:
7 days = 62.0%
14 days = 94.2%
21 days = 87.3%
28 days = 114.7%
The test substance degraded >60% in the 10 day window. The reference substance, aniline degraded by 89% after 28 days.
**Test condition:** Total solids concentration of the inoculum: not determined
Test volume: 80 ml
Temperature: 22 +/- 1 C
pH: 6.94 - 7.49.
**Reliability:** (2) valid with restrictions
Test is comparable to guideline study, although some experimental
details are not reported.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (92)

**Type:** aerobic
**Inoculum:** other: no information on inoculum provided
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 60 % after 30 day(s)
**Result:** inherently biodegradable
**Kinetic:**
4 day(s) = 39 %
10 day(s) = 53 %
17 day(s) = 57 %
24 day(s) = 59 %
31 day(s) = 60 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) except that dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the
solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** There is no information given on the validity criteria.
**Result:** Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation during the test period.
**Reliability:** (4) not assignable
The information reported is insufficient to assess the validity of this study.
11-OCT-2005 (123)

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 10 mg/l related to COD (Chemical Oxygen Demand)
**Degradation:** = 59 % after 29 day(s)
**Result:** inherently biodegradable
**Kinetic:** 3 day(s) = 15 %
8 day(s) = 43 %
15 day(s) = 52 %
29 day(s) = 59 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A five-day bacterial inhibition test was performed under the conditions of the Closed Bottle Test. In this preliminary test, the test material was degraded to 27% of its COD. In a subsequent Modified Sturm Test, the test material was added to two vessels containing mineral salts medium and activated sludge to give a nominal test concentration of 10 mgC/L. Controls vessels comprised two containing inoculated mineral salts medium alone and one containing inoculated mineral salts medium plus sodium benzoate (positive control). Test and control vessels were aerated for 29 days with air treated to remove CO2.
**Remark:** Cumulative CO2 production in the controls after 29 days (77.8 and 80.1 mgCO2) was within the acceptable range for
this assay system (recommended maximum = 120 mgCO2 for a three litre culture). The reference compound reached the pass level within 14 days and the parallel assays did not differ by more than 20%. No information is given on total
inorganic carbon levels at the start of the test.

Mean cumulative CO2 production by the mixtures containing the test substance at 10 mgC/L was equivalent to 15% after three days and 59% after 29 days.

**Result:** Kinetic of control substance:
3 days = 39%
8 days = 74%
15 days = 82%
29 days = 89%
The test substance degraded <60% over the test period and therefore cannot be considered readily biodegradable. However, significant degradation was observed therefore the substance is considered inherently biodegradable.

**Test condition:** Total solids concentration of inoculum: 30 mg/l
Temperature: 21.2 - 23.9°C
pH: 7.4 - 7.6

**Reliability:** (2) valid with restrictions
Guideline study although some validation data not reported.

17-OCT-2005 (58)

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 50 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 30 day(s)
**Degradation:** = 65 - 77 % after 30 day(s)
**Result:** readily biodegradable

**Method:** other: RDA-Blok-Test equivalent to a two-phase closed bottle test
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The method used is suitable for poorly water-soluble compounds. No information is provided regarding the validity criteria.
This information is from a summary of the full report and reports test concentration as 100 mg COD/l in the test procedure and 50 mg COD/l in the results section.

**Result:** 15 days = 30-75%
30 days = 65-77%
Degradation data only reported for days 15 and 30.

**Reliability:** (4) not assignable
Summary report only available. There is insufficient information reported to assess the validity of this test

30-AUG-2005 (53)

**Type:** aerobic
**Inoculum:** activated sludge

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The inoculum used was activated sludge from a semi-continuous colony maintained in the laboratory.
Incubation was carried out at 25°C in 200 ml Erlenmeyer flasks containing 5 ul of a alcohol and 100 ml of culture medium.

Biodegradation rate constant was determined by measurement ofalcohol concentration in the supernatant of the culture by gas chromatography.

**Result:** The biodegradation rate constant for 1-octanol was 0.36 hr-1.This equates to a half-life of 1.9 hours.
**Reliability:** (2) valid with restrictions
Non-guideline study.
30-AUG-2005 (128)

**Type:** anaerobic
**Inoculum:** other: digested sewage sludge diluted to 10%

**Method:** other
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Sludge was collected from primary or secondary anaerobic digesters. The method used digested sewage sludge diluted to 10% and incubated anaerobically in 160 ml serum bottles with 50 ug of C per ml of test chemical. Biodegradation was determined by the net increase in gas pressure in bottles with test chemicals over the pressure in nonamended sludge bottles. Gas production was measured by gas chromatography and by a pressure transducer. Compounds were incubated for 8 weeks.
**Result:** Octanol was readily mineralized (> 75% of theoretical methane production).
**Test condition:** Concentration of inoculum: 10% diluted sludge
Test volume: not reported
Temperature: 35 C
pH: not reported
**Reliability:** (2) valid with restrictions
Non-guideline study
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (102)

**Type:** aerobic
**Inoculum:** activated sludge, adapted
**Concentration:** 2 mg/l related to Test substance
**Degradation:** = 100 % after 30 day(s)

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Test condition:** Biologically hard emulsifier used (Nonylphenol 10 EO/5 PO).
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
10-JAN-2005 (48)

**Type:** aerobic
**Inoculum:** other: municipal sewage treatment plant effluent
**Concentration:** 5 mg/l
**Degradation:** = 55 %

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Test condition:** Biologically hard emulsifier used (Nonylphenol 10 EO/5 PO).
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
10-JAN-2005 (48)

**Type:** anaerobic
**Inoculum:** anaerobic sludge
**Concentration:** 50 mg/l related to Test substance

**Method:** ECETOC Anaerobic biodegradation
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Mean degradation rate for 70 day test period was 64.6 +- 19.2 %
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
10-JAN-2005 (49)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**GLP:** no data
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.

BOD was determined by measurement of dissolved oxygen concentrations in the test vessels at the start and end of the test period.
**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.

**Result:** 54.1% degradation after 5 days (% ThOD)
**Test substance:** As prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
Non-guideline study
17-OCT-2005 (117)

**Method:** other: Assessed using methods based on OECD Guideline 301D (Closed Bottle Test) and Procedure C.4-E of the Annex to Directive 92/69/EEC
**GLP:** no data
**Year:** 1996
**Method:** Triplicate mixtures containing the test substance at nominal concentrations of 6.8 mg/L and 3.4 mg/L in mineral salts medium inoculated with final effluent from a sewage treatment plant were incubated for 5 days. The COD of the test material was determined by oxidation with an acid-dichromate mixture using a semi-micro procedure, in which Cr(VI)is reduced to Cr (III).
**Result:** The mean BOD after 5 days was 1.50 gO2/g. The mean COD was 2.43 gO2/g. The BOD:COD ratio ranged from 49% to 74%.
The mean 5 day BOD of Kalcohl 0898 was 62% of its COD.
**Test condition:** Concentration of inoculum: 5 ml/l
Test volume: not reported
Temperature: 20.2-20.9 C
pH: 6.6-7.5
**Test substance:** As prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
17-OCT-2005 (59)

## 3.7 Bioaccumulation

**BCF:** = 95

**Method:** other: calculated (Veith et al, 1979)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 3.15 was used in the calculation
**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (5)

## 3.8 Additional Remarks

**Memo:** Additional environmental fate/exposure summary for octanol (111-87-5)

**Remark:** Octanol is released to the environment as a natural constituent of plants and microbes. It may also be released to the environment through effluents at sites where it is produced or used in perfumery, cosmetics, organic synthesis, solvent manufacturing of high boiling esters, antifoaming agents and in food flavoring. Photolysis or hydrolysis of octanol is not expected to be environmentally important. Octanol should biodegrade rapidly in soil and water. Differing estimates of Koc indicate a wide range of adsorption characterisitcs for octanol and the mobility class in soil may range from low to high; it may partition from the water column to organic matter in sediments and suspended solids. The potential for bioconcentration of octanol in aquatic organisms is low. The volatilization half-lives from a model river and a model pond, the latter of which considers the effect of adsorption, have been estimated to be about 1.8 and 82 days, respectively. Octanol is expected to exist entirely in the vapor phase in ambient air. Vapor-phase reactions with photochemically produced hydroxyl radicals in the atmosphere may be important (estimated half-life of 1.3 days). Physical removal from air via precipitation has been shown to occur. The most probable human exposure to octanol would be occupational exposure, which may occur through dermal contact or inhalation at places where it is produced or used. Common non-occupational exposures would include the ingestion of foods containing it.

**Reliability:** (4) not assignable
Textbook used for background information.

10-JAN-2005 (55)

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 13.3 - 13.5
**Limit Test:** no

**Method:** other: ASTM 1980.
**Year:** 1983
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Both Veith et al. (1983a and 1983b) citations have the same authors and report the same data. In addition, the results appear to be repeated in the studies by Brooke et al. 1984 and Broderius and Kahl 1985. Veith reports results for juveniles, Brooke reports results for fry and Broderius reports results for both. Broderius has been chosen as the representative study as this provides the most detail with regard to test results. The publications indicate that test concentrations were monitored daily using analytical methods, however the results are not provided.

**Result:** RESULTS: EXPOSED
LC50 = 13.3 (12.6 - 14.4) mg/l for fry
LC50 = 13.5 (12.2 - 15.0) mg/l for juveniles
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: No control mortality in tests with juveniles and less than 10% in tests with fry (refers to all 27 chemicals tested in study)

**Test condition:** TEST ORGANISMS
Strain: Fathead minnow
Supplier: Not reported
Age: Newly hatched fry were < 24 hours old and juvenile fathead minnows 28 to 34 days old
Weight: 0.12 g (juveniles)
Feeding: Spawning stock and juveniles were cultured on recently hatched brine shrimp nauplii (Artemia sp.) and frozen adult brine shrimp
Pretreatment: Acclimated to test chambers for 2-3 hours prior to introduction of toxicants
Feeding during test: none
Control group: 1 control group (5 fish)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle/solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: Aeration in head water reservoirs
Alkalinity: 44.0 mg/l as CaCO3
Hardness: 44.6 mg/l
Conductance: not reported
TEST SYSTEM

Concentrations: not reported
Renewal of test solution: water replacement 2-4 h (25 ml/min)
Exposure vessel type: Glass chambers with silicone sealant
Number of replicates: 1
Fish per replicate: 5
Test temperature: 25 C
Dissolved oxygen: > 80% saturation
pH mean: 7.6
Adjustment of pH: not reported
Intensity of irradiation: 22 to 38 lumens/sq ft
Photoperiod: Illuminated with wide spectrum fluorescent bulbs for 16 h daily
TEST PARAMETER: lethality
SAMPLING: mortalities recorded daily
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported but publication indicates daily analytical monitoring was conducted

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
19-JUL-2005 (29) (30) (120) (121)

**Type:** semistatic
**Species:** Alburnus alburnus (Fish, estuary)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 16
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
The earlier study reports the LC50 = 15-17 mg/l
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available
19-JUL-2005 (19) (77)

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC0:** = 10
**LC50:** = 17
**LC100:** = 30
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
**Remark:** This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. The test method used corresponds to OECD Guideline 203. Mortalities were recorded at 24 hour intervals.
**Reliability:** (2) valid with restrictions
20-OCT-2005 (52)

**Type:** static
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = 3.2
**LC50:** = 18
**Limit Test:** no

**Method:** other
**Year:** 1996
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** In this preliminary toxic screen, groups of five fish were exposed to the test substance at nominal concentrations of 0.1, 0.32, 1, 3.2, 10, 32, and 100 mg/L. Control groups of fish were placed into dilution water alone or dilution water containing HCO-40 at the same level as in the test medium at the highest concentration. Observations of the fish were made on at least 24-hour intervals.
**Result:** Sublethal, treatment-related effects were noted at 10 mg/L and higher concentrations and included hyperventilation, darkened pigmentation, lethargy and loss of coordination. All affected fish showed symptoms within 15 minutes of exposure.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
19-JUL-2005 (60)

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** = 8
**LC50:** = 16
**LC100:** = 33

**Method:** other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf

**Remark:** Toxicity tested in two different laboratories under comparable conditions; data of Luedemann.
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were

reported for the test results to be reliably assigned to the CAS number.

17-OCT-2005 (69)

**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC50:** = 17.7

**Method:** other: No particulars of test method given.

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.

17-OCT-2005 (80)

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** 16
**LC50:** 20
**LC100:** 23

**Method:** other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf

**Remark:** Toxicity tested in two different laboratories under comparable conditions; data of Juhnke.
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.

20-OCT-2005 (69)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 15 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC0:** = 6.8
**EC50:** = 20
**EC100:** = 71
**Limit Test:** no

**Method:** other:
**Year:** 1982
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
EC0: 6.8 mg/l
EC50: 20 (15-26) mg/l
E100: 71 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24hrs old
Feeding: Dry algae
Pretreatment: None
Feeding during test: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF THE TEST CHEMICAL SOLUTIONS: no analysis
DILUTION WATER
Source: Standardised synthetic fresh water
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Range of test concentrations to achieve three or more responses between 0 and 100%
Renewal of test solution: none
Exposure vessel type: 50 ml flask
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: oxygen saturated
pH mean: 7.6 - 7.7
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 9 hours artificial lighting
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:

None
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
19-JUL-2005 (28)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = 19
**EC50:** = 26
**Limit Test:** no

**Method:** other
**Year:** 1989
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This acute 24 hour daphnia test was carried out prior to a 21 day reproduction test in daphnia. No information is given on the test conditions.
The nominal concentrations were given as no results of chemical analysis were available for the 24 hour EC50.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with higher toxicity values are available.
19-JUL-2005 (74)

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 58
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available
19-JUL-2005 (19) (77)

**Species:** Daphnia magna (Crustacea)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 36.6
**Limit Test:** no

**Method:** other: standard
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The LC50 reported here (36.6 mg/L) reflects a mean of two other studies; 47 mg/L reported in Bringmann and Kuhn 1977 and 26 mg/L reported in Burton 1992. Bringmann and Kuhn 1977 study was superceded by Bringmann and Kuhn 1982 which reported a lower EC50. The Burton 1992 study is not available.
**Reliability:** (4) not assignable
Not key study: This result is a secondary report from two previous studies.
19-JUL-2005 (22) (33) (112)

**Species:** other: Ceriodaphnia dubia
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 8.7

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study. This result is a secondary report from Burton 1992 which is not available. No details are available.
19-JUL-2005 (33) (112)

**Species:** Gammarus sp. (Crustacea)

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** 4 - 40 min EC50 = 6.3 - 7.2 mg/l
**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
19-JUL-2005 (122)

**Type:** static
**Species:** other: Tubifex tubifex (Oligochaeta)
**Exposure period:** 3 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 190
**Limit Test:** no

**Method:** other
**Year:** 1997
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Test media were prepared by dilution of a stock solution. The acute immobilisation test was carried out under static conditions. The EC50 was based on counting the number of worms that stopped moving within 3 minutes of exposure to test medium.
**Reliability:** (4) not assignable
Documentation insufficient for assessment. Information obtained from the open literature. Only a brief description of the test method is given.
09-SEP-2005 (94)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 25 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC10:** = 2.8 - 4.2
**EC50:** = 6.5 - 14
**Limit Test:** no

**Method:** other
**Year:** 1989
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Modified Test Procedure incorporating DIN 38 412, Part 9 and account also being taken of the Test Methods using Water Organisms, DIN 38 412, Part 1.
**Result:** RESULTS: EXPOSED
Biomass EbC50 = 6.5 mg/l
Growth rate ErC50 = 14 mg/l
Based on nominal concentrations
**Reliability:** (4) not assignable
Documentation insufficient for assessment.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (74)

**Species:** other algae: Enteromorpha intestinalis
**Endpoint:** other: ion retention
**Exposure period:** 2 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 120
**Limit Test:** no

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Samples of E. intestinalis comprising several pieces of thallus from different specimens (total weight 1 g) were risnsed once in distilled water for 3 seconds then placed in 50 ml of distilled water in a beaker and left for 2 min (sample 1). The E. intestinalis was then transferred to lidded bottles containing a further 50 ml of distilled water then placed in a boiling water bath. After 5 min the bottles were removed from the bath and the contents poured through a plastic sieve into a 100 ml beaker (sample 2). The alga was discarded. The conductivity of samples 1 and 2 was measured and used to derive an ion retention health index. This index reflects the proportion of the total leechable ions present in the thallus which were retained after exposure to distilled water for 2 mins. The index was calculated by dividing the conductivity of sample 2 by the total conductivity (i.e.sample 1 + sample 2).
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with lower effect concentrations are available.
21-OCT-2005 (98)

**Species:** Scenedesmus quadricauda (Algae)
**Endpoint:** biomass
**Exposure period:** 8 day(s)
**Unit:** mg/l **Analytical monitoring:** no data
**Toxicity Threshold (TT) :**
= 6.3
**Limit Test:** no

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (3) invalid
It is not possible to determine if exponential growth was maintained throughout the test.
21-OCT-2005 (26) (27)

**Species:** Microcystis aeruginosa (Algae, blue, cyanobacteria)
**Endpoint:** biomass
**Exposure period:** 8 day(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT :** = 1.9
**Limit Test:** no

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Tested in the cell multiplication inhibition test. The concentration of the algal suspension of each test culture was measured turbidimetrically and expressed as the

extinction of the primary light of the monochromatic radiation at 578 nm for a 10 nm layer. Control cultures were monitored over the 8 day exposure period.
Toxicity threshold is the pollutant concentration causing the onset of cell multiplication inhibition.

**Result:** RESULTS: EXPOSED
TT = 3.5 mg/l
Based on measured results

**Test condition:** TEST ORGANISMS
Strain: Microcytis aeruginosa
Source/Supplier: Not reported
Pretreatment: None
Controls: 12 control cultures containing algal suspension, stock nutrient solution and bidistilled water under sterile conditions
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Not reported
Concentration of vehicle, solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Standard algal medium
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Not reported
Renewal of test solution: Not reported
Exposure vessel type: Culture tubes stoppered with cotton-lined metal caps
Number of replicates: 3
Initial cell concentration: Quantity of cell material used for inoculation is determined turbidimetrically and is standardised.
Test temperature: 27 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: To neutral if required
Intensity of irradiation: Not reported
Photoperiod: Exposed to constant lighting by luminescent tubes (Osram L 40/30)2 in a central field between two lateral luminescent tubes at 60 cm distance from each other.
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

**Reliability:** (3) invalid
It is not possible to determine if exponential growth was maintained throughout the test.

21-OCT-2005 (25)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other protozoa: Entosiphon sulcatum
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT or EC3 :** = 44

**Method:** other
**Year:** 1980

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Dissolved toxic water ingredients will inhibit cell multiplication of the protozoan, Entosiphon sulcatum. Thus, in a test culture containg dissolved toxic substances the count of organisms, after a certain period will be less than in a test culture kept under identical conditions, however, free from toxic influence. The number of protozoa is determined by means of a cell counter.
**Test condition:** TEST ORGANISMS
Strain: Entosiphon sulcatum
Supplier: Stock cultures
Feeding: Bacteria, Escherichia coli
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: Not reported
Vehicle, solvent: Not reported
Purity/supplier: Not reported
DILUTION WATER
Source: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Not reported
Dosing rate: Not reported
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 2
Test temperature: 25 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: None
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported
**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.
19-JUL-2005 (27)

**Species:** Photobacterium phosphoreum (Bacteria)
**Exposure period:** 15 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 4.7 - 6

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
19-JUL-2005 (122)

**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 33 - 51

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available

19-JUL-2005 (122)

**Species:** Uronema parduzci (Protozoa)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 23

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
19-JUL-2005 (122)

**Species:** other bacteria: Clostridium acetobutylicum (anaerobic)
**Exposure period:** 6 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 130

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
19-JUL-2005 (122)

**Species:** other bacteria: Clostridium botulinum (anaerobic)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 200

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
19-JUL-2005 (122)

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 100

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
**Reliability:** (3) invalid
09-SEP-2005 (46)

**Type:** aquatic

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 16 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**TT or EC3 :** > 50

**Method:** other: static cell multiplication inhibition test
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Toxic threshold concentration = concentration at which optical density of
culture is > 3 % below control value
**Source:** Henkel KGaA Duesseldorf
**Test condition:** T = 25 degr. C; cell growth determined photometrically (436 nm)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005

**Species:** activated sludge
**Unit:** mmol/l **Analytical monitoring:**
**EC50:** = 2.5

**Method:** other: Flow microcalorimetry toxicity test
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 2.5 mmol/l = 325.6 mg/l
parameter: reduction in heat flux (measured with flow microcalorimeter)
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** T = 25 degr. C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (15)

**Species:** activated sludge
**Exposure period:** 3 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** 350

**Method:** other: OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test''
**Year:** 1984
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess

the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

11-OCT-2005 (110)

**Species:** activated sludge
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** 200

**Method:** other: Serum bottle toxicity test according to Blum, D.J.W., doctoral thesis presented to Drexel University, Philadelphia, Pa. (1989)
**Year:** 1989
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** parameter: cumulative oxygen consumption over a period of 24 h
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** : assay in sealed tubes; T = 25 degr. C; gently shaken
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

11-OCT-2005 (110)

**Species:** Bacillus subtilis (Bacteria)
**Unit:** mmol/l **Analytical monitoring:**
**EC50:** = 4

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 0.4 mmol/l = 52.1 mg/l. Parameter: inhibition of initial germination rate at 37
degr. C in phosphate buffer measured as reduction in absorbance at 650 nm pH 7.2
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** Methanol as solvent (in concentrations not exceeding its minimum inhibitory conc. of 0.2 M)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available

11-OCT-2005 (127)

**Species:** Chilomonas paramaecium (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**TGK 5% :** > 20

**Method:** other: cell multiplication inhibition test (static)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** cell multiplication measured with cell counter
TGK = toxische Grenzkonzentration (toxic threshold concentration); concentration at which optical density of culture is 5 % below control value
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** T = 20 degr. C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (24)

**Species:** Photobacterium phosphoreum (Bacteria)
**Exposure period:** 15 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** 6

**Method:** other: Bioluminescence test (Microtox test
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (32)

**Species:** Photobacterium phosphoreum (Bacteria)
**Exposure period:** 5 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 5.93

**Method:** other: Bioluminescence test (Microtox test) according to Beckman Instruments Manual
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (111)

**Species:** Photobacterium phosphoreum (Bacteria)
**Exposure period:** 5 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** 6.3

**Method:** other: Bioluminescence test (Microtox test) according to Beckman Instruments Manual

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available
11-OCT-2005 (35)

**Species:** Photobacterium phosphoreum (Bacteria)
**Exposure period:** 15 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** = 4.73

**Method:** other: Bioluminescence test (Microtox test) according to Beckman Instruments Manual
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available
11-OCT-2005 (54)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** 3000
**EC10:** 10000

**Method:** other: Pseudomonas-Atmungs-Hemmtest, DIN 38412 Teil 27, in Vorbereitung, "Bestimmung der Hemmwirkung von Abwasser auf die Sauerstoffzehrung von Pseudomonas putida."
**Test substance:** as prescribed by 1.1 - 1.4

11-OCT-2005

**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EC50:** = 32.69 - 51.05

**Method:** other: static test
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** analysis of actual test substance concentration by GC
cell growth photometrically determined (540 nm)
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess

the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available

11-OCT-2005 (99)

**Species:** Uronema parduzci (Protozoa)
**Exposure period:** 20 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**TGK 5% :** = 23

**Method:** other: cell multiplication inhibition test (static)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** cell multiplication measured with cell counter
TGK = toxische Grenzkonzentration (toxic threshold concentration); concentration at which optical density of culture is 5 % below control value.
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** T = 25 degr. C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available

11-OCT-2005 (23)

**Species:** other bacteria: Clostridium acetobutylicum
**Exposure period:** 6 hour(s)
**Unit:** mmol/l **Analytical monitoring:**
**EC50:** 1

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 1 mmol/l = 130.26 mg/l
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** anaerobic conditions; 35 degr. C; growth monitored hourly by direct optical density measurements at 620 nm
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available

11-OCT-2005 (65)

**Species:** other bacteria: Clostridium botulinum
**Unit:** mg/l **Analytical monitoring:**
**MIC :** = 200

**Method:** other: static cell growth inhibition test according to Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
**Year:** 1975
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test duration not mentioned

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** anaerobic conditions; cell growth (turbidity) visually determined
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available
11-OCT-2005 (57)

**Species:** other bacteria: mixed microbial culture
**Exposure period:** 75 minute(s)
**Unit:** mol/l **Analytical monitoring:**
**EC50:** = .0048

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 0.0048 mmol/l = 625 mg/l
Origin of microbial culture not specified. Culture adapted to growth on test substance prior to test.
Parameter: Oxygen consumption at 30 degr. C measured manometrically
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available
11-OCT-2005 (116)

**Species:** other fungi: see remarks

**Method:** other: test for inhibition of spore germination
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parameter: inhibition of spore germination
Species: no antifungal activity up to:
---
Aspergillus niger 1000 mg/l (5 d; 28 degr. C; pH 5.6)
Trichoderma viride 1000 mg/l ( " )
Trichophyton
mentagrophytes 100 mg/l ( " )
Myrotecium verrucaria 1000 mg/l ( " )
Candida albicans 100 mg/l (20 h; 37 degr. C; pH 5.6)
Mucor mucedo 1000 mg/l ( " )
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess

the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (43)

**Species:** other protozoa: Tetrahymena elliotti
**Exposure period:** 90 minute(s)
**Unit:** mmol/l **Analytical monitoring:**
**MIC :** = 1.585

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** MIC: 1.585 mmol/l = 162 mg/l
microscopical evaluation of cell movement (paramenter: MIC = lowest concentration to give complete cessation of movement)
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** incubation for 90 min. at room temperature
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (12)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

**Species:** Pimephales promelas (Fish, fresh water)
**Endpoint:** other: survival of young fish
**Exposure period:** 7 day(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** = 1.5 - 11.9
**LOEC:** = 3 - 11.9

**Method:** other: U.S. EPA 1000.0
**Year:** 1995
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** In addition to 1-d old larvae, 4- and 7-day old larvae were also used.
**Remark:** The primary focus of this study was to determine if there is a statistical difference in using older larvae for this test method. Survival, growth, and biomass endpoints were recorded. Note that this study utilizes the 7-day short-term test method and therefore is not technically a "chronic" fish study. However, the method is commonly used to estimate the sensitivity of early life stages of fish to chemicals and efluents.
The toxicity was not affected by the age of the larvae.
**Result:** RESULTS: EXPOSED
Survival
NOEC = 1.5 - 11.9 mg/l
LOEC = 3.0 - 11.9 mg/l
Growth
NOEC = 0.75 - 3.0 mg/l

LOEC = 1.5 - 6.0 mg/l
Based on nominal loading rates
RESULTS: CONTROL
Three side by side exposures were conducted with 1-octanol because survival of 1-d control larvae in the first set was only 78%, which is less than the acceptable criteria of 80% or greater control survival. However, the 1-d larvae test was analysed by declaring one of the replicates an outlier because only 1 larvae of 10 survived, while survival was 100% in the other three control replicates.

**Test condition:** TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Fathead minnow culture unit at the EPA Newtown Facility
Post-hatch transfer time: 12 hours
Age: 1, 4 and 7 day larvae
Feeding: Larvae were fed 3 drops per replicate of concentrated brine shrimp slurry. The larvae were fed once on the first day, twice daily on days 1 to 6 and not fed on the last day.
Control group: 1 control group (4 replicates each containing 10 larvae)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle/solvent: none
DILUTION WATER
Source: Prepared with reagant grade chemicals added to a carbon-filtered, deionised Cincinnati tap water that was treated in a Millipore Milli-Q system
Aeration: Aerated vigorously for approx. 24 hours before usage
Alkalinity: 56 - 64 mg/l
Hardness: 86 - 94 mg/l
Conductance: not reported
TEST SYSTEM
Concentrations: 0.75, 1.5, 3.0, 6.0 and 11.9 mg/l
Renewal of test solution: not reported
Exposure vessel type: 600 ml borosilicate glass beakers
Number of replicates: 4 replicates per test concentration
Fish per replicate: 10
Test temperature: 25 +/- 1 C
Dissolved oxygen: Mean = 6.0 mg/l (4.4-7.2 mg/l)
pH mean: 7.5 (7.24-7.81)
TEST PARAMETER: survival and growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: 3 grab samples were taken of the final test solution and the measured concentration of the high concentration (11.9 mg/l) was 1.3 mg/l. Grab samples of final concentrations of 6.0 and 3.0 mg/l gave measured concentrations of 0.09 mg/l and none detected.

**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.

19-JUL-2005 (91)

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Mortality, reproduction rate, and appearance of offspring

**Exposure period:** 21 day(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = 1

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Recommendation of the German Federal Environmental Agency on the Performance of Testing according to Sec 5, Para 1, No. 3 of the Regulation on Application Documents and Evidence under the Chemicals Act.
**Remark:** Primarily, the results were expressed with reference to the nominal concentration. If however, the chemical analysis showed a loss of tested substance greater than 20% , then the lowest analysed concentration (minimum value) obtained during the test was also given for the NOEC.
The 21-d NOEC based on nominal concentrations was 1.6 mg/l.
The 21-d NOEC based on the minimum value for 1-Octanol was 1.0 mg/l.
**Result:** RESULTS: EXPOSED
21d NOEC = 1.6 mg/l (based on nominal value)
21d NOEC = 1.0 mg/l (based on measured value)
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: 24 hours old
Feeding: Tetramin-Hauptfutter (fish feed) and activated sludge were used as feeds, daphnia fed daily.
Control group: 1 control group (4 replicates, five animals per replicate)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle/solvent: none
DILUTION WATER
Source: Deionised water
Aeration: Aerated up to the water saturation level
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 0.4 to 50 mg/l
Renewal of test solution: Parent animals in test and control vessels were pipetted 3 times a week (Mondays, Wednesdays and Fridays) into freshly prepared test and control media
Exposure vessel type: 400 ml beakers
Number of replicates: 4 per concentration
Animals per replicate: 5
Test temperature: 25 +/- 1 C
Dissolved oxygen: Average minimum oxygen saturation value of 69% was measured at the end of the test period (related to all test substances in test)
pH mean: >7
TEST PARAMETER: mortality, reproduction rate and appearance of offspring
MONITORING OF TEST SUBSTANCE CONCENTRATION: Samples were taken twice from selected concentration levels of the test

series during the test period and analysed chemically.
**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.
19-JUL-2005 (75)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**Species:** other: Bursaphelenchus lignicolus (pine wood nematode)
**Exposure period:** 24 hour(s)
**Unit:** other: mg/l
**LC0:** = 130
**LC100:** = 1302

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
19-JUL-2005 (122)

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble

fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (38)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:

n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.

No further information on other biotransformation pathways of these alcohols was provided.

**Source:** Kamil et al, 1953
Hayes Consultancy Service Bromley, Kent

**Test condition:** These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including C6-C18 alcohols included in this category, form glucuronic acid conjugates in the rabbit.

Groups of 3 Chinchilla rabbits, about 3 kg in weight, were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.

The results were reported as the amount of extra glucuronic acid excreted as a % of dose.

**Test substance:** n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol

**Conclusion:** All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (71)

**Result:** The publication reported in full the results only for lauryl aclohol arriving at a value for the expiratory excretion rate which was the ratio of amount of compound excreted via expired air to the amount absorbed. It was 91% for lauryl alcohol. The respiratory excretion rates for all the other alcohols investigated were >65% although the actual data is not reported. Following skin application of lauryl alcohol about 2.84 % of the administered dose was absorbed. Of this absorbed dose >90% was excreted in expired air (CO2).

Absorption decreased with increasing carbon chain length. The absorption rate was investigated in different solvents (squalene, castor oil, triethyl citrate (TEC). The percutaneous absorption rate of undiluted n-octanol was 50%, this was increased in squalene but decreased in castor oil or

TEC. This was also reported with the other alcohols tested and the tendency was more pronounced at higher concentrations.

The degree of skin irritation was proportionally related to the degree of percutaneous absorption.

**Source:** Iwata et al, 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 3 hairless mice were used to investigate percutaneous absorption of various an-alkanols ncluding n-octanol. The 1-C14 labelled test substances were applied to the dorsal skin using a plaster for a 24 hour period. Immediately following application each animal was placed in a container to measure expiratory excretion. At the end of the exposure period the treated area of skin was excised and dissolved using tissue solubiliser. The carcass was homogenised in a blender wwith sodium hydroxide. An aliquot of the homogenate was then dried and combusted for determination of radioactivity.

The effect of different solvents and concentration of the solvent was also investigated. The role of skin irritation in absorption of test substance was examined.

**Test substance:** n-octyl alcohol; n-decyl alcohol, lauryl alcohol and cetyl alcohol all radiolabelled (1-C14) and >98% pure.

**Conclusion:** At least 65% of the absorbed dose is excreted as CO2 in the expired air. Absorption decreased with increasing carbon chain length and was affected by solvent and concentration.

**Flag:** Critical study for SIDS endpoint

09-SEP-2004 (64)

**Remark:** 1-octanol is oxidised to octanal which is rapidly oxidised to octanoic acid. Octanoic acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Test substance:** As prescribed 1-octanol

**Reliability:** (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including 1-octanol.

11-NOV-2004 (125)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: Holtzman albino
**Sex:** male/female
**No. of Animals:** 60
**Vehicle:** other: undiluted
**Doses:** 4680, 6600, 9330, 13170, 18600, and 26280 mg/kg bw
**Value:** = 18240 mg/kg bw

**Method:** other: not specified
**Year:** 1965
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All deaths occured within 24 hours of dsoing.
- Number of deaths at each dose: 0/10, 0/10, 1/10, 0/10, 5/10, 8/10

CLINICAL SIGNS: On the day of dosing, diarrhea, weakness, ataxia and malaise were observed in most of the animals at the four highest test levels. Animals which did not die overnight returned to normal within 6 days, most within 2 days.

NECROPSY FINDINGS: Most animals which died had pulmonary and adrenal congestion. Some also had slight congestion of the stomach. In the sacrificed animals, weight gains were in the normal limits and gross necropsy did not reveal any remarkable findings. At the highest dose level, bloody encrustations about the nares were evident.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported, mortality was presented as a combined value so no independent assessment can be made.

**Source:** Scientific Associates, Inc. 1965b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS:
- Source: No data
- Weight at study initiation: data given but document illegible at this point.
- Group size 5M+5F
- Controls: no

ADMINISTRATION:
- Doses: 1.17, 1.65, 2.33, 3.28, 4.64 and 6.55 gm/kg
- Doses per time period: not reported
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during the observation period. Body weights of survivors were recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

**Test substance:** Tradename Alfol 8.

**Conclusion:** The rat oral LD50 value (M+F) for Alfol 8 was 18.24 g/kg confidence limits 14.25 to 23.34 g/kg. No specific target organ was identified.

**Reliability:** (2) valid with restrictions
Well documented and conducted study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

16-JUL-2005 (100)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female

**No. of Animals:** 10
**Vehicle:** other: as an aqueous suspension
**Doses:** 5 g/kg single dose level
**Value:** > 5000 mg/kg bw

**Method:** other: OECD 401 (limit test)
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no deaths during the course of the study.

CLINICAL SIGNS: During the first 24 hours all test animals showed some decrease in actvity and piloerection. The animals showed a gain in body weight at all measurement points during the 14 day observation period.

NECROPSY FINDINGS: The were no abnormal findings.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: No.

**Source:** Henkel KGaA 1981a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Winkelmann, Hanover, Germany
- Weight at study initiation: mean body weight males, 137, females 127
- Group size: 5M+5F
- Controls: no

ADMINISTRATION: Gavage animals fasted
- Doses: 5 g/kg
- Doses per time period: single dose
- Volume administered or concentration: administered as a 25% aqueous suspension at a constant volume of 20 ml/kg.
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were observed particularly during the first 24 hours after dosing. Body weights were recorded prior to dosing and at 24 hours, 1 week and 2 weeks after dosing. All survivors were subject to gross necropsy at the end of the observation period.

**Test substance:** Tradename Lorol 8
**Conclusion:** The rat oral LD50 for Lorol 8 was >5g/kg when applied as an aqueous suspension. Clinical signs of intoxication were confined to slight sedation and piloerection during the first 24 hours following dosing. There was no remarkable gross pathology at necrospy and no indication of specific target organ toxicity.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Well documented and conducted study.
**Flag:** Critical study for SIDS endpoint
16-JUL-2005 (50) (62)

**Type:** LD50
**Species:** rat
**Strain:** other: no data

**Sex:** no data
**Value:** > 3200 mg/kg bw

**Method:** other
**GLP:** no
**Test substance:** other TS: 2-octanol

**Remark:** This value is reported in several secondary references as being the LD50 value for n-octanol. These sources are erroneous, the original report in Patty 1963 of an unpublished reference by Fassett is clearly a value for 2-octanol. This value does not appear in Patty 2001.
**Reliability:** (4) not assignable
Secondary reference.
14-SEP-2004 (62) (88) (93)

**Type:** LD50
**Species:** rat
**Value:** > 5000 mg/kg bw

**Method:** other: no data
**Year:** 1973
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of unpublished data from Levenstein, 1972 report to RIFM.
**Reliability:** (4) not assignable
Secondary reference.
14-SEP-2004 (62) (88) (90)

**Type:** LD50
**Species:** rat
**Value:** = 20000 mg/kg bw

**Year:** 1984
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unspecified changes in the brain, liver and urinary system, no indication of dose level.
**Reliability:** (4) not assignable
Secondary reference to Russian language original, unobtainable.
17-OCT-2004 (93)

**Type:** LD50
**Species:** mouse
**Value:** = 1790 mg/kg bw

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of an unobtainable Russian study reported by RTECS.
**Reliability:** (4) not assignable
Secondary reference.
07-OCT-2004 (62) (93)

**Type:** LD50
**Species:** mouse
**Value:** = 15000 mg/kg bw

**Year:** 1984
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unspecified changes in the brain, liver and urinary system, no indication of dose level.
**Reliability:** (4) not assignable
Secondary reference to Russian language original, unobtainable.
17-OCT-2004 (93)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 25
**Vehicle:** other: air
**Doses:** 5600 mg/m3
**Exposure time:** 4 hour(s)
**Value:** > 5600 mg/m³

**Method:** other: in house protocol
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Report in Patty of unpublished data from Amoco. No deaths were observed among rats exposed to 6400 mg/m3 (1203 ppm) for 1 hour. 2/10 rats died within 2 hours of a 4 hour exposure to 5600 mg/m3 (1053 ppm). Necrosis of the bronchial epithelium with alveolar oedema and infiltration of alveolar macrophages was observed. No details of the incidence.
**Result:** MORTALITY: There were no deaths following 1 hour exposure to 6.39 mg/l 1-octanol.

Following 4 hour exposure to 5.6 mg/l. 3/5 male rats died following the 4 hour exposure all females survived:
- Time of death: 1-2 days after exposure.

CLINICAL SIGNS: Salivation and gasping or rapid respiration were observed during and/or immediately after each exposure. Other signs of intoxication included inactivity, rales, coldness, redness around the eys and nose, ocular opacity and exophthalmus and anogenital staining.

BODY WEIGHT: All exposed rats lost body weight following exposure, the survivors of the 4 hour exsoure did not regain weight until day 6 of the exposure period.

NECROPSY FINDINGS: On gross examination treatment related findings were confined to the lungs.

1 hour exposure: lesions described as foci/discoloured areas were observed in 3/5 males and 2/5 females.

4 hour exposure: lesions described as foci/discoloured areas were observed in 4/5 males and 4/5 females. All lungs appeared oedematous.
Controls: 1 male had lung foci.

Histopathological examination of the lungs of rats exposed for one hour revealed no microscopic lesions other than minimal alveolar heamorrhage in 1 male. Lungs from control rats were unremarkable. In animals exposed for 4 hours microscopic lesions included necrosis of the bronchial epithelium (4/5M, 2/5F), alveolar oedema (4/5M, 4/5F) with accumulation of alveolar macrophages (10/10), congestion (2/5M, 1/5F), alveolar haemorrhage (1/5M, 1/5F), regeneration of the bronchial epithelium (2/5M, 3/5F) and alveolar hyperplasia (1/5F).

POTENTIAL TARGET ORGANS: Lungs

SEX-SPECIFIC DIFFERENCES: Males more susceptible.

**Conclusion:** The 4 hour rat LC50 for 1-octanol is >5.6 mg/l (nominal). There were clinical signs of respiratory distress and histopathological evidence of irritation of the respiratory tract.

**Test condition:** TEST ORGANISMS: Rat, SD
- Source: Charles River, Portage, MI, USA
- Age: 6 weeks
- Weight at study initiation: (mean weights) males 340g; females 236g
- Group size: 5M+5F treated
- Controls: 2M+2F untreated

ADMINISTRATION: Inhalation
- Doses: 5.6 mg/l for 4 hours; 6.39 mg/l for 1 hour (nominal conc.) There was no analytical monitoring of the vapour conentration.
- Atmosphere generation: the test substance was heated to approx. 425C and and the resultant vapour administered to the animals in a whole body inhalation chamber.
- Post dose observation period: 7 days

EXAMINATIONS: Clinical observations were made throughout exposure, on removal from the exposure chambers and at least once daily throughout the observation period. Bodyweights of the treated animals were recorded prior to exposure and prior to necropsy. All test and control animals were subject ot gross necropsy and the lungs were examined histopathologically.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment with restrictions, no measurement of concentration.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (2) (90) (93)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white

**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: undiluted test substance
**Doses:** 1, 2 and 4 g/kg
**Value:** = 2000 - 4000 mg/kg bw

**Method:** other: contract laboratory protocol
**Year:** 1976
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All deaths occurred within 4 days of exposure.
- Number of deaths at each dose: Intact skin 0/2, 1/4 and 2/2, abraded skin 0/2, 3/4 and 2/2.

LD50(s): Intact skin: 2-4 g/kg; Abraded skin: 1-2 g/kg; combined intact and abraded 2 g/kg. A visual assessment of test site suggested that >75% of the dose was observed at each dose level.

APPLICATION SITE: At the end of the exposure period all animals showed slight to severe erythema and oedema particulary of the ventral skin and particularly in animals with abraded skin. In all survivors wrinkling and coreaceousness gradually developed forming and inelastic sheath around the trunk of the animal. The healing process continued throughout the 14 day observation period.

CLINICAL SIGNS: Generalised weakness and inactivity in most animals following exposure. Survivors appeared normal at 72 hours post exposure. These signs persisted and/or intensified in animals which eventually died. Final body weights of surviving animals showed moderate to severe loss in 2 animals, constant weight in 3 animals, and slight to moderate gain in 3 animals.

NECROPSY FINDINGS: In animals which succumbed there was severe skin damage with maceration and erosion of the ventral skin and musculature. Blanching and multiple focal haemorrhages of the gastric mucosa, friability of the liver, moderate heamaturia and a slight accumulation of amber, watery peritoneal fluid were observed internally.

Rabbits surviving to 14 days showed moderate to marked desquamation, severe erosion and multiple focal haemorrhages of the gastric mucosa and slight accumulation of clear or amber viscous fluid in the peritoneal cavity.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

**Source:** Scientific Associates, Inc. 1976a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3 - 2.9 kg

- Group size: low dose and high dose 2M+2F and mid dose 4M+4F half with intact skin the others with abraded skin.
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2 and 4 g/kg
- Removal of test substance: Excess material removed with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

**Conclusion:** The rabbit dermal LD50 for Alfol 8 following 24 hour occlusive exposure was 2000-4000 mg/kg. There was significant evidence of skin irritation at the application site persisting in some animals throughout the observation period. Clinical signs were indicative of a general toxic effect coupled with anorexia. The most common gross pathogical finding was erosion of the gastric mucosa.

**Reliability:** (2) valid with restrictions
Study reasonably well conducted and reported. Particularly where the skin was abraded the degree of irritation reported at the contact site (full depth erosion) may have contributed to the death of the animals.

**Flag:** Critical study for SIDS endpoint

14-SEP-2004 (101)

**Type:** LD50
**Species:** rabbit
**Value:** > 5000 mg/kg bw

**Year:** 1972
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of unpublished data from Levenstein, 1972 report to RIFM.

**Reliability:** (4) not assignable
Secondary reference.

14-SEP-2004 (62) (88) (90) (93)

**Type:** LD50
**Species:** guinea pig
**Value:** > 500 mg/kg bw

**Year:** 1972
**Test substance:** other TS: 2-octanol

**Remark:** This value is reported in several secondary references as being the LD50 value for n-octanol. These sources are erroneous, the original report in Patty 1963 of an unpublished

reference by Fassett is clearly a value for 2-octanol. This value does not appear in Patty 2001.

**Reliability:** (4) not assignable
Secondary reference.

14-SEP-2004 (62) (88) (93)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** other: none
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual mean 24+48+72 hour scores 1.0, 2.0 and 1.3. Group mean 24+48+72 hour score 1.43.
- Edema: All scores 0.

REVERSIBILITY: By day 7 all erythema and oedema scores were 0.

OTHER EFFECTS: The test site was sticky to touch at 1 hour post-dosing. A loss of elasticity at the test site was reported at 48 and 72 hours. From day 7 until the end of the observation period (day 16) exfoliation was observed in all test animals. Control sites showed no skin irritation all scores 0.

**Source:** Johnson 1996a; OECD 1987b.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.22 - 2.64 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 3X2 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 16 day
- Controls: The other flank of the animal was used as a control site.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours post application then at 7, 10, 13 and 16 days.

**Conclusion:** The C8 alcohol Kalcohl 0898 is not a skin irritant according to either EU criteria following a 4 hour semi-occlusive exposure. Kalcohl 0898 can be considered as a mild irritant under GHS criteria.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (67)

**Species:** other: rabbit, guineapig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: vaseline

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** other TS: even C6-22 alcohols

**Result:** Result : The most marked skin reactions were observed with

rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in some Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).

1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test substance was applied at 50% in vaseline. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

**Reliability:** (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

18-OCT-2004 (62) (70)

**Remark:** This report of skin irritation with n-octanol is reported in several secondary references. These sources are erroneous, the original report in Patty 1963 of an unpublished reference by Fassett is clearly an assessment for 2-octanol. This data does not appear in Patty 2001.

**Test substance:** 2-octanol

**Reliability:** (4) not assignable
Secondary reference.

17-OCT-2004 (62) (88) (93)

**Remark:** Undiluted C8-alcohol applied undiluted to intact or abraded rabbit skin was reported to produce mild skin irritation. No further experimental details were available from this secondary reference to unpublished data provided by

Levenstein, 1972.
**Source:** Opdyke, 1973a
**Test substance:** Reported as a C8 alcohol (1-octanol)
**Reliability:** (4) not assignable
Secondary reference.
11-NOV-2004 (89) (93)

**Remark:** 2% 1-octanol in petrolatum did not cuse irritation to human skin following a 48 hour closed application. 25 volunteers were tested. No further details available from this secondary report of unpublished data provided by Kligman, 1972.
**Test substance:** 1-octanol
**Reliability:** (4) not assignable
Secondary reference.
11-NOV-2004 (89) (90)

### 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** irritating
**EC classificat.:** risk of serious damage to eyes

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hr mean)
- Cornea: Individual scores 2, 1, 1 (group mean 1.33)
- Iris: All 1 (group mean 1)
- Conjuntivae (Redness): 2.3, 1.7, 1.3 (group mean 1.8)
- Conjuntivae (Chemosis): 1, 1.3, 0.7 (group mean 1)

DESCRIPTION OF LESIONS: Iritis, slight to moderate conjuncitivitis and areas of very slight/slight corneal opacity during the first 72 hours. Very slight conjunctivitis observed in all 3 animals at days 8 and 15.

REVERSIBILITY: Very slight conjunctivitis persisted in 2 animals until termination on day 22. Iritis persisted in one of these rabbits until day 22.

OTHER EFFECTS: Blepharitis of the lower lid seen in 2 rabbits at 72 hours persisting to day 8 in one rabbit. Very slight/slight initial pain response.
**Source:** Johnson 1996d
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK

- Age: 5 months
- Weight at study initiation: 2.88 - 3.13 kg
- Number of animals: 3
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 22 days

EXAMINATIONS
- Scoring system: As prescribed in OECD test method.
- Observation period: 22 days
- Tool used to assess score: Ophthalmoscope or pencil beam tourch. Fluorescein used from 24 hours onward as required to aid corneal examination.

**Test substance:** Tradename Kalcol 0898

**Conclusion:** Kalcol 0898 is an eye irritant according to EU criteria based on individual mean 24+48+72 hour scores for iritis of >= 1 in all test animals. This material is considered a category 1 eye irritant under GHS and to cause a risk of serious damage to eyes (EU) based on persistence of iritis (1 rabbit) and conjunctivitis (2 rabbits) to 22 days.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (68)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: Individual 1, 2, 2 Mean 1.7
- Iris: Individual 0, 1, 1 Mean 0.7
- Conjunctivae (Redness): Individual 1.7, 2.3, 2.7 Mean 2.2
- Conjunctivae (Chemosis): Individual 1.7, 3, 2.7 Mean 2.5
- Overall irritation score: MMAS (modified maximum average score) 41.0

REVERSIBILITY: Complete reversal in 14 days for all 3 test animals, 1 eye appeared normal after 7 days.

**Source:** ECETOC, 1998

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Unspecified
- Source: No data

ADMINISTRATION/EXPOSURE

- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 21 days

EXAMINATIONS
- Ophthalmoscopic examination: No data
- Scoring system: No data
- Observation period: 1, 24, 48, 72 hours, 7, 10, 14 and 21 days (assessments made until the test eye for each animal showed complete reversal to normal up to 21 days)
- Tool used to assess score: No data

The study was included as part of a data base of in vivo eye irritation results. All studies were conducted to OECD guideline under GLP.

**Conclusion:** 1-octanol is classifiable as an eye irritant based on scores of =>2 for corneal opacity, =>1 for iritis and =>2 for chemosis. The lesions were reversible within 14 days. According to GHS criteria 1-hexanol is a Class 2A irritant based on individual mean 24+48+72 hour scores in at least 2 test animals of => 1 for corneal opacity and iritis and => 2 in at least 2 test animals for conjunctival chemosis and redness.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

16-JUL-2005 (39)

**Species:** other: New Zealand White albino rabbits
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE mean 24+48+72hr (96 hour mean)
- Cornea: 2.23 (2)
- Iris: 0.7 (0.5)
- Conjuntivae (Redness): 2.57 (2)
- Conjuntivae (Chemosis): 1.9 (1)

Individual scores were not reported.

DESCRIPTION OF LESIONS: none given.

REVERSIBILITY: The observation period was 96 hours. At this time point mean scores had reduced for all parameters as indicated in parentheses above.

OTHER EFFECTS: The mean surface of corneal damage was reported this was at a maximum of 75% at 24 hours reducing to 5% at 96 hours.

**Source:** Jacobs 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbits
- Strain: New Zealand White
- Sex: no data
- Source: no data
- Number of animals: 6
- Controls: no

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 96 hours

EXAMINATIONS
- Ophthalmoscopic examination:
- Scoring system: Draize
- Observation period: 96 hours
- Tool used to assess score: 2% sodium fluorescein before visual scoring of % corneal damage

**Conclusion:** 1-octanol is an eye irritant according to EU criteria based on a mean 24+48+72 hour score for 6 rabbits of 2.57 for conjuctivitis and 2.23 for corneal opacity. Results are only given up to 96 hours post instillation but the evidence was that the effects were reversing at this time point. Lack of individual scores precludes accurate assessment by GHS however based on the mean scores of 6 rabbits for corneal opacity of 2.23 and for iritis of 0.7 and given the evidence of reversibility 1-octanol is considered a Category 2A eye irritant.

Cited in Iuclid 2000 and Patty 2001.

**Reliability:** (2) valid with restrictions
Guideline study without detailed information.

**Flag:** Critical study for SIDS endpoint

11-NOV-2004 (62) (66) (90)

## 5.3 Sensitization

**Type:** other:maximisation test
**Species:** other: man
**No. of Animals:** 25
**Vehicle:** petrolatum
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: Kligman human maximization test
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This reference gives a summary report of unpublished data provided by Kligman 1972.

Also cited in Iuclid 2000 and Patty 2001.

**Result:** Under the conditions of this test 1-octanol was not a human skin sensitiser.

**Source:** Opdyke, 1973.

Hayes Consultancy Service Bromley, Kent
**Test condition:** This patch test was carried out using the maximization procedure described by Kligman, A.M.the identification of contact allergens by human assay. III The maximization test: A procedure for screening and rating contact allergens. J. Invest. Dermatol. 47:393-409, 1966. There are variations in this procedure but we have no information as to which variation was used. The exposure would have been a 48 hour occlusive exposure and sodium lauryl sulphate may have been used to promote the response. The only experimental detail given for 1-octanol was that a panel of 25 volunteers were tested at a concentration of 2% in petrolatum. there is no indication as to whether this was an induction or challenge concentration.
**Reliability:** (4) not assignable
Secondary reference.
11-NOV-2004 (62) (88) (90)

## 5.4 Repeated Dose Toxicity

-

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames Test)
**System of testing:** Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
**Concentration:** 4, 20, 100, 500, and 2500 ug/plate
**Cytotoxic Concentration:** 2500 ug/plate for all strains, 500 ug/plate for some strains (see text)
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: An in-house protocol similar to OECD No. 471
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls showed an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested also at 500 ug/plate for strains TA1537, 1538 and 98.
- Without metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested also at 500 ug/plate for strains TA1538 and 98.
**Source:** Henkel KGaA 1982a
Hayes Consultancy Service Bromley, Kent
**Test condition:** METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in

reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate suspended in Tween 80/aqueous
- Number of replicates: Four per dose level.
- Application: Plate incorporation.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

**Test substance:** Tradename Lorol C8

**Conclusion:** The C8 alcohol Lorol C8 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Cytotoxicity was observed at the highest dose level tested.

Cited in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (limited reporting).

**Flag:** Critical study for SIDS endpoint

16-JUL-2005 (51) (62)

**Type:** other: Bacterial reverse mutation assay (Ames test)
**System of testing:** Salmonella typhimurium strains TA98 and TA100
**Concentration:** 50, 158, 500, 1580, 5000 ug/plate
**Cytotoxic Concentration:** No cytotoxicity observed.
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: Ames
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: no increase in reverse mutation rate in any of the treated groups. Positve controls showed an appropriate increase in mutation rate.

PRECIPITATION CONCENTRATION: none reported.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: none observed at the highest test concentration of 5000 ug/plate.

**Source:** Huntingdon Life Sciences Ltd 1996k.
Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING

- Species/cell type: Salmonella typhimurium strains TA98 and TA100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced.

ADMINISTRATION:
- Dosing: 50, 158, 500, 1580 and 5000 ug/plate.
- Number of replicates: Duplicate
- Application: Pour plate, solvent DMSO.
- Positive and negative control groups and treatment: Negative controls DMSO and untreated bacterial control. Positive controls benzo[a]pyrene 5 ug/plate, sodium azide 2 ug/plate, 2-nitrofluorene 1 ug/plate.
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: not reported

**Test substance:** Tradename Kalcol 0898

**Conclusion:** The C8 alcohol Kalkohl 0898 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 5000 ug/plate.

**Reliability:** (2) valid with restrictions
Ames test no protocol specified but similar OECD 471 using only 2 tester strains. Criteria for evaluation were not reported.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (61)

**Type:** other
**System of testing:** Chinese hamster V79 cells
**Concentration:** 0.8 mmoles/l

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Survival was 71% in the test cultures at 30 minutes. The number of cells with >22 chromosomes after 3 hours exposure to 1-octanol was 10.9% in the test group [20/183] compared to 25/500 and 29/592 in the control groups (5 and 4.9 % respectively). The significance of this increase was $p<0.01$. As cell survival decreased, c-mitosis increased. Based on the dose response observed for the induction of c-mitosis and aneugenicity and together with the cytotoxicity profile the authors concluded that the effects on spindle function of highly lipophilic compounds including 1-octanol was most likely induced through an indirect (physical) mechanism relating to the partitioning of the test substance into cellular hydrophobic compartments and not related to a direct interaction with spindle formation and function.

**Test condition:** In this investigative study to determine markers for aneugenicity, 10(6) Chinese hamster lung cells (V79) were seeded for measurements of cell survival, aneuploidy and c-mitotic activity and cultured for 20-24 hours prior to treatment with the test substance. Incubation with the test substance (conc. 0.8 mmoles/l) was for 30 minutes (c-mitosis, survival) or 3 hours (aneuploidy). Following treatment the slides were fixed, dried and stained. Normal and affected

metaphases, anaphases and iclophases were scored for c-mitosis (100 mitotic cells/slide, 2 slides per dose for each experiment. Only those metaphases (100-200/slide) with 21 or more chromosomes were scored for aneuploidy. The authors note that 1-octanol was poorly soluble in water and that the addition of acetone to aid solubility was not successful resulting in precipitation of the test substance.

**Conclusion:** This investigative study into markers for potential aneugenicity showed that 1-octanol caused increased aneuploidy and C mitosis. The study authors noted that for the aliphatic alcohols the threshold for the aneugenic responses and the cytotoxicity were very close and concluded that the observed effects reflected physico-chemical interactions rather than a true indication of potential genotoxicity

Cited by RTECS, 2004

**Reliability:** (3) invalid
There is no information presented to verify that adequate quality assurance methods were in place to ensure that the test system functioned appropriately. Presently, in-vitro assays to detect aneuploidy rely on more sensitive, alternative methods and the validity of the data presented in this study are therefore uncertain (ECETOC Monograph 27, Aneuploidy, 1997).

29-DEC-2005 (87) (93)

## 5.6 Genetic Toxicity 'in Vivo'

**Type:** Cytogenetic assay
**Species:** rat **Sex:** male
**Strain:** other: unspecified
**Route of admin.:** other: intragastric
**Exposure period:** 48 hours
**Doses:** 1/5th LD50
**Result:** ambiguous

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:
600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 1.0 +-0.4
Cells with breakages %: controls 0.3 +-0.2; treated 1.0 +-0.4;
Cells with chromosome aberrations %: controls 0; treated 2.6 +-0.7.

STATISTICAL RESULTS: Reported as above.

**Source:** Barilyak, 1988

**Test condition:** TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage
- Vehicle: Homogenised emulsion
- Duration of test: 48 hours
- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Conclusion:** Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability:** (3) invalid
Significant methodological deficiences (see test conditions).

15-SEP-2004 (13)

**Type:** Sister chromatid exchange assay
**Species:** Chinese hamster **Sex:** no data
**Route of admin.:** i.p.

**Method:** other: in vivo sister chromatid exchange
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no increase in sister chromatid exchange in the cells treated with 1-octanol alone, the level of SCE (3.0 +_0.1 SCE/cell) was comparable with controls (2.9 +-0.2 SCE/cell). When injected in the presence of NMU 1-octanol reduced the incidence of SCE seen with NMU alone.
**Test condition:** 1-octanol prepared as an emulsion in saline was injected intraperitoneally into a single Chinese hamster aged between 12-13 weeks of age and weighing ca 30g at a dose level of 10(-3) moles/kg bw. 2 control animals received an injection of water. All animals received a subcutaneous implant of BrdU in the neck prior to treatment and injection of colchicine 2 hours before sacrifice at 24 hours. 50 cells from the control animals and 25 from the treated animals were scored for induction of SCE. The study was carried out as part of an investigation of the effects of n-alkanols on the induction of SCE by NMU and NMU acted as a positive control.
**Reliability:** (3) invalid
Significant methodological deficiencies, use of only one test animal limits the validity of this study. In the secondary publication by Tucker et al, 1993 this study is considered as inadequate or equivocal.
07-OCT-2004 (108) (113)

**Remark:** In common with other members of the aliphatic alcohols category C6-12 alcohols (Types A,B,C and D) contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the range of category members (linear and essentially linear), including a negative Ames test for 1-octanol, are negative. Results from in vivo studies with other category members and/or supporting substances provide evidence that these alcohols are not genotoxic in vivo.

Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (104) (105) (119)

## 5.7 Carcinogenicity

**Species:** mouse **Sex:** male/female
**Strain:** other: A/He
**Route of administration:** i.p.
**Exposure period:** 8 weeks
**Frequency of treatment:** 3 injections per week for 8 weeks
**Post exposure period:** 16 weeks
**Doses:** maximum tolerated dose (MTD) and 1:5 dilution of MTD

**Result:** negative
**Control Group:** yes

**Method:** other: mouse pulmonary tumour system
**Year:** 1972
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY AND TIME TO DEATH: See below for survival, time of death was not reported.

BODY WEIGHT GAIN: Measured but not reported.

LUNG TUMOUR INCIDENCE:

1-octanol:

| Total Dose (g/kg) | Sex | Survivors | No. mice with tumors | No. of tumors/ mouse |
|---|---|---|---|---|
| 12 | M | 14/15 | 2 | 0.21 |
| 12 | F | 13/15 | 3 | 0.13 |
| 2.4 | M | 13/15 | 1 | 0.08 |
| 2.4 | F | 14/15 | 4 | 0.36 |

The occurrence of lung tumors in the vehicle (tricaprylin purified) control was 0.24 tumors/mouse for males and 0.2 for females. The occurrence in untreated mice was males 0.22 and females 0.17 tumours/mouse. There was no statistically significant treatment related increase in the incidence of lung tumours with 1-octanol. In the positive controls the number of tumours/mouse at the low dose level (10 mg/kg) was 10.5 and 9.1 in males and females respectively and double this at the high dose level (20 mg/kg).

There was no treatent related occurrence of tumours in other tissues examined.
**Source:** Stoner et al. 1973.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Age: 6-8 weeks
- Weight at study initiation: 18 - 20g
- Number of animals: 15M+15F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: The mice were injected thrice weekly for 8 weeks.
- Type of exposure: Intra-peritoneal.
- Post exposure period: 16 weeks
- Vehicle: Tricaprylin (purified)
- Concentration in vehicle: Not reported
- Total volume applied: 0.1 ml/mouse
- Doses: Total dose of either 2.4 or 12 g/mouse based on preliminary range finding these equate to 1/5 MTD and the MTD. An untreated and positive control group (urethan 5 or 20 mg/mouse) was included.

CLINICAL OBSERVATIONS AND FREQUENCY
- Body weight: twice weekly during dosing, monthly thereafter.

- Food & water consumption: Not reported
- Clinical signs: Not reported
- Mortality: Frequency of observations not reported.
- Macroscopic examination: At 24 weeks.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Lungs, liver, kidney, spleen, thymus, intestine, salivary and endocrine glands were examined for abnormalities.
- Microscopic: Some of the lung tumours were taken for histopathological examination. Lungs were also evaluated for other abnormalities including inflammatory reactions and adenomatosis.

OTHER EXAMINATIONS: The numbers of tumours on the lung surface were counted.

STATISTICAL METHODS: Tumour incidence in treated vs controls was compared by the standard X2 test.

**Conclusion:** In the A mouse pulmonary tumour system neither 1-octanol nor 1-dodecanol showed any potential to increase the incidence of lung tumours following repeated intraperitoneal injection.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (62) (90) (109)

**Species:** mouse **Sex:** female
**Strain:** Swiss
**Route of administration:** dermal
**Exposure period:** 60 weeks
**Frequency of treatment:** three times weekly
**Post exposure period:** none
**Doses:** 4 ug/mouse in cyclohexane
**Result:** negative
**Control Group:** no

**Method:** other: skin tumour promotion study
**Year:** 1966
**GLP:** no data
**Test substance:** other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.

**Source:** Sice 1966.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane
- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)
- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Test substance:** The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Conclusion:** In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application site in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999).

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (8) (85) (86) (90) (103)

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol

category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C8 (1-octanol) alcohol is not expected to impair fertility are provided by lack of observed effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C) and similar negative data from the supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for reproductive toxicity are based are either comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (104) (106) (119)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Species:** rat **Sex:** female
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** gestation days 6-15
**Frequency of treatment:** daily
**Duration of test:** 20 days
**Doses:** 0, 130, 650, 975, and 1,300 mg/kg/day
**Control Group:** yes
**NOAEL Maternal Toxity:** = 130 mg/kg bw
**NOAEL Teratogenicity:** = 1300 mg/kg bw

**Method:** other: Closely followed EEC directives 87/302/EEC and 67/548/EEC and OECD Guideline No. 414
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Divergence from test method by using 10 animals/group instead of 20.
**Result:** NOAEL: The NOAEL for maternal toxicity is 130 mg/kg/day based on overt maternal toxicity at higher dose levels. There were no treatment related effects on the foetus and the NOAEL for teratogencity and foetotoxicity is 1300 mg/kg.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 130, 650, 975 and 1300 mg/kg/day (some problems with the detection method suggest that the actual dose administered at the top dose levels may have been larger than the nominal value)

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: Two dams died in the top dose group (1300 mg/kg/day) and a further 2 in the 650 mg/kg/day group.
- Number pregnant per dose level: water control 9, aqueous emulsifier 10, 130 mg/kg 10, 650 mg/kg 9, 975 mg/kg 8, 1300

mg/kg 8.
- Number aborting: None
- Number of resorptions: Comparable in treated and control groups. Resorptions (all)/dam (mean) 1.0, 1.4 (controls); 1.2, 0.7, 0.8 and 1.3 treated groups low - high.
- Number of implantations: Comparable in treated and control groups. Implantation site/dam (mean) 14.7, 16.0 (controls); 14.7, 15.4, 13.8 and 14.5 treated groups low - high.
- Post implantation loss: Comparable in treated and control groups.
- Number of corpora lutea: Comparable in treated and control groups. Corpora lutea/dam (mean)14.8, 16.3 (controls); 15.0, 16.0, 14.9 and 14.5 treated groups low - high.
- Duration of Pregnancy: Comparable in treated and control groups.
- Body weight: A slight decrease in body weight gain in the 650, 975 and 1300 mg/kg treated groups from day 15 to the end of the study was not of statistical significance.
- Food/water consumption: A slight decrease (magnitude not reported) in food consumption was reported in the 650, 975 and 1300 mg/kg treated groups.
- Description, severity, time of onset and duration of clinical signs: There was a dose related increase in signs of maternal toxicity observed at all dose levels with increasing severity. The effects at the lowest dose level 130 mg/kg/day were marginal. Signs observed were assumption of a lateral or abdominal position, piloerection, unsteady gait, salivation, nasal discharge and pneumonia.
- Hematological findings incidence and severity: not carried out
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not reported
- Organ weight changes: Uterine weight and placental was unaffected by treatment.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable in treated and control groups.
- Number viable: Viability was comparable to controls. Live foetuses/dam (mean) 13.7, 14.6 (controls); 13.5, 14.7, 13.0 and 13.2 treated groups low to high.
- Sex ratio: Not reported.
- Total malformations, variations and retardations: The incidence was unaffected by treatment. All foetal values were within the range of biological variation. Differences in malformations or retardations were not statistically significant and without dose relationship. A single cheiloschisis and one anophthalmy in the top dose group were considered incidental and not related to treatment. Litters with malformations number (%) 2 (22), 3 (30) (controls); 3 (30), 3 (43), 2 (25) and 1 (17) treated groups low to high. Litters with variations number (%) 8 (89), 10 (100) (controls); 10 (100), 7 (100); 7 (88) and 5 (83) treated groups low to high. Litters with retardations number (%) 8 (89), 9 (90) (controls); 9 (90), 7 (100), 8 (100) and 5 (83) treated groups low to high.

**Source:** Hellwig and Jackh 1997
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Groups of 8-10 pregnant Wistar rats aged 68-85 days at study initiation, mean weight 214-233 g

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage
- Duration of test/exposure: treatment day 6-15 post coital, termination day 20 post coital.
- Treatment: 130, 650, 975 and 1300 mg/kg/day
- Control group and treatment: two control groups were used one with twice distilled water and one with 0.005% Cremophor EL as emulsifier.
- Vehicle: 0.005% Cremophor in water
- Concentration in vehicle: Adjusted to give constant volume
- Total volume applied: 5 ml/kg

MATING PROCEDURES: 1 fertile male to 4 females.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Daily
- Clinical observations: Daily
- Examination of uterine content: At gestation day 20, uterine weight, numbers of implantations shown as: live foetuses, dead implantations, early resorptions (stained), early & late resorptions (unnstained), dead foetuses. Conception rates and pre & post implantational losses were calculated.
- Examination of fetuses: Foetal weights, external, visceral and skeletal anomalies, variations & retardations, unclassified observations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC): Not reported

STATISTICAL METHODS: Dunnetts test for most reproductive parameters and Fischers exact test for evaluaton of conception rate and all foetal findings.

**Conclusion:** Administration of n-octanol to pregnant female rats by gavage on gestation days 6-15 caused dose related overt clinical signs of toxicity (irritation and transient CNS depression) at dose levels in excess of 130 mg/kg/day. However there were no treatment related effects on the offspring or reproductive parameters monitored and the NOAEL for teratogenicity and foetotoxicity is 1300 mg/kg/day with a maternal NOAEL of 130 mg/kg/day.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (Group sizes are smaller than recommended 8-10 pregnant females rather than 20).

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (47)

**Species:** rat **Sex:** female
**Strain:** Sprague-Dawley
**Route of administration:** inhalation
**Exposure period:** 19 days
**Frequency of treatment:** 7 hours/day
**Duration of test:** 20 days
**Doses:** 400 mg/m3

**Control Group:** yes
**NOAEL Maternal Toxity:** > .4 mg/l
**NOAEL Teratogenicity:** > .4 mg/l

**Method:** other: see text
**Year:** 1990
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The results reported in the primary reference (Nelson et al, 1990) are summarised in a comparative review of 13 alcohols tested by the same author (Nelson et al, 1996). The test concentration for n-octanol is apparently misquoted in Nelson 1990b as the original reference gives the test concentration as 400 mg/m3. The erroneous value (350 mg/m3) is carried through to Patty 2001.

**Result:** NOAEL : 0.4 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotoxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5% of the nominal concentration of 0.4 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study. Actual dose achieved 0.402 mg/l.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: Comparable in treated and control groups. Mean resorptions/litter control 0.5, treated 0.4.
- Number of corpora lutea: Comparable between treatd and control groups. Mean corpora lutea/litter control 14.0, treated 14.8.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Comparable between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Litter weights control males 3.22g, females 3.12g; treated males 3.56g, females 3.44g.
- Sex ratio: No significant difference between treated and controls. Control males/litter 6.6, females 6.9; treated males 5.9, females 7.9.
- External, Soft tissue and Skeletal abnormalities: No treatment related effects. Data not presented.

**Source:** Nelson et al. 1990
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
Groups of approximately 15 female pregnant Sprague-Dawley rats with a mean maternal weight of 257 g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose level: 0.4 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F. Control animals were sham exposed.

MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC): Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA. Foetal incidence data were analysed using the Variance Test for Homogeneity of the Binomial Distribution or ANOVA. The Kruskal-Wallis test was used if a non-parametric analysis was more appropriate.

**Conclusion:** The NOAEL for maternal toxicity, foetotoxicity and teratogenicity in rats following inhalation exposure to n-octanol during gestation (Gestation days 1-19) is >0.4 mg/l (the highest attainable concentration). There were no adverse effects on any of the maternal or foetal parameters investigated.

Cited in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (62) (83) (84)

**Species:** other: Chick embryo **Sex:**
**Route of administration:** other: Injected suprablastodermically
**Frequency of treatment:** once
**Doses:** 0.05M
**Control Group:** other: olive oil

**Method:** other: see text
**Year:** 1979
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** N-octanol showed no significant teratological potential compared to the control group. Malformations were observed in 6.45% of the n-octanol treated embryos vs 7.9% of the controls.

**Source:** Forschmidt et al. 1979
Hayes Consultancy Service Bromley, Kent

**Test condition:** Very little experimental detail available in the abstract report of this study. Up to 50 chick embryos were injected at 72 hours of incubation. The potential teratogenic effectof the test material on the embryos was compared to a solvent control group (olive oil).

**Reliability:** (4) not assignable
Abstract

15-SEP-2004 (41)

## 5.8.3 Toxicity to Reproduction, Other Studies

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## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

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## 5.11 Additional Remarks

**Type:** other: human skin irritation method development

**Result:** Hexanol and octanol gave responses significantly lower than the positive control and results were similar between laboratories. These alcohols were therefore not considered as skin irritants.

Decanol gave equivocal responses, an initial test gave a response just sufficient to classify as irritant. Subsequent testing by 3 other laboratories did not confirm this result.

**Source:** Griffiths et al, 1997
Hayes Consultancy Service Bromley, Kent

**Test condition:** These materials were tested as part of an interlaboratory evaluation of a human patch test for identification of skin irritation potential.

Groups of at least 30 volunteers were used for each evaluation at each location, at least 2 locations tested each product. The undiluted material (0.2 ml) was applied to the outer arm using a Hill Top chamber for a period usually of 4 hours. the reaction was assessed at 24, 48 and 72 hours after initiation of the exposure. SDS (sodium dodecyl sulphate) was used as a positive control. If the proportion of the test group reacting to the test material was significantly less that those reacting to the positive control the material was considered as not classifiable as a skin irritant.

**Test substance:** hexanol, octanol, decanol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

16-JUL-2005 (44)

**Type:** other: human skin irritation method development

**Remark:** The purpose of this study was to compare the nitrocellulose-replica method (24 hour semi-occlusive exposure to the flexor surface of the arms) with closed patch testing (24 hour application to the back in a Finn chamber, 15 ul test material). The study was based on 20 healthy volunteers.

The results evaluated using the closed patch testing showed that skin irritation for octanol significantly increased with increasing concentration of the test compound. Lauryl, cetyl and stearyl alcohols were of low irritancy. However the nitrocellulose-replica method could detect skin irritation with the higher alcohols which was not observed in the closed patch testing.

**Source:** Sato et al, 1996
Hayes Consultancy Service Bromley, Kent

**Test substance:** octyl alcohol, lauryl alcohol, cetyl alcohol, stearyl alcohol.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

15-SEP-2004 (96)

**Type:** other: aspiration hazard

**Remark:** Aspiration of 0.2 ml 1-octanol to rats produced deaths in 10/10 rats after a few breaths.

**Test substance:** n-octanol

**Conclusion:** In this screening test 1-octanol presents an aspiration hazard.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

15-SEP-2004 (42) (90)

**Type:** other: sensory irritation

**Remark:** The RD50 for 1-octanol was reported as 50 ppm in Swiss mice. Exposure time not reported. The original paper (Muller & Greff, 1984) reports unpublished data which is summarised in Bos et al, 1992.

**Test substance:** 1-octanol

**Reliability:** (2) valid with restrictions
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11-NOV-2004 (20) (82)

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 112-30-1 |
| **CAS No.** | 112-30-1 |
| **EINECS Name** | decan-1-ol |
| **EC No.** | 203-956-9 |
| **TSCA Name** | 1-Decanol |
| **Molecular Formula** | C10H22O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 30-JUN-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **106** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK, The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

02-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium Member
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 20138 Milano
**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Olefins and Surfactants GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** Paul-Baumann-Strasse, 1
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza, PO box 4320
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
02-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

02-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Decanol
**Smiles Code:** OCCCCCCCCCC
**Mol. Formula:** C10 H22 O1
**Mol. Weight:** 158.29

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-decanol, CAS 112-30-1 are 100% linear.

The substance comprises >90% C10. Components of even chain length, in the range C8-C12 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms , including a selection of commercial product names, are:
1-Decanol (9CI) (CA INDEX NAME)
Decyl alcohol (8CI)
Kalcohl 10H
n-Decanol
n-Decyl alcohol
Nacol 10
Nacol 10-99
Nafol 10
Nonylcarbinol
NSC 406313
Royaltac
Sipol L 10
T 148
Alcohol C-10
Capric alcohol
Decan-1-ol
Alfol 10 Alcohol
Some commercial products with the name CO

Some commercial products with the name Lorol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-decanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca >25 000 - 50 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >50 000 000 - 100 000 000 pounds.

Japan: Production 7000 tonnes, consumption 13 000 tonnes (alcohols in range C6-11)-
This is publicly-available CEH data for Japan, for 2001.

21-DEC-2005 (93)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 2 Adhesive, binding agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 10 colouring agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 10 colouring agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Paints, lacquers and varnishes.
19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Surface Treatment
19-SEP-2005

**Use category:** 50 Surface-active agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, the remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, the remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site

limited).
19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.
21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification 1. ID No. 71.
05-AUG-2005 (102)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-decanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
02-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

02-AUG-2005

## 2.1 Melting Point

**Value:** = 6.4 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (20) (63)

**Value:** = -7 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (100)

**Value:** = 6.9 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
03-JAN-2005 (87)

**Value:** = 3 - 6 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (75)

**Value:** = 4 - 7 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (75)

**Value:** = 7 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
03-JAN-2005 (14)

## 2.2 Boiling Point

**Value:** = 229 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (14)

**Value:** = 231 - 234 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment.
03-JAN-2005 (28) (63)

**Value:** = 220 - 235 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (75)

**Value:** = 220 - 240 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (75)

## 2.3 Density

**Type:** density

**Value:** = .8297 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (14)

**Value:** = .83

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (100)

**Type:** density
**Value:** = .82 - .83 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (75)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0113 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
05-OCT-2005 (22)

**Value:** = 2.93 hPa at 91 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (100)

**Value:** = 1.33 hPa at 69.5 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
03-JAN-2005 (61)

**Value:** = 293 at 90.9 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference cited is an authoritative, peer-reviewed
secondary data source
03-JAN-2005 (14)

**Value:** = .012 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
09-AUG-2005 (2)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 4.57

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
valid with restrictions Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for octanol-water partition coefficient values.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (32)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 39.5 mg/l

**Method:** other: measured

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for water solubility values.
**Flag:** Critical study for SIDS endpoint
03-JAN-2005 (104)

**Solubility in:** Water
**Value:** = 7.97 mg/l at 20 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
03-JAN-2005 (60)

**Solubility in:** Water
**Value:** = 106 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
03-JAN-2005 (88)

**Solubility in:** Water
**Value:** = 37 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
03-JAN-2005 (12) (87)

**Solubility in:** Water
**Value:** = 39.5 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 39.5 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

09-AUG-2005 (2)

**Solubility in:** Water
**Value:** = 40 mg/l at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
21-SEP-2005 (13)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 82 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Although not stated, this is considered likely to be a result from a closed-cup test by comparison with other values.
**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
03-JAN-2005 (96)

**Value:** ca. 110 degree C
**Type:** open cup

**Method:** other: DIN ISO 2592
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (75)

**Value:** ca. 110 degree C
**Type:** open cup

**Method:** other: DIN 51758
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
03-JAN-2005 (75)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (54)

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (54)

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
03-JAN-2005

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (54)

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM.

03-JAN-2005

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 15.36831E-12 cm3/molecule.sec
Half-life: 25.1 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
21-DEC-2005 (4)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
09-SEP-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 158.3
Data temperature 25 deg C
Log Kow 4.57
Water Solubility 39.5 mg/l
Vapour pressure 1.13 Pa

Melting point 6.4 deg C
half life in air 25.1 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 2.57% |
| Soil | 92.5% |
| Water | 2.81% |
| Fish | 5.22E-03% |
| Sediment | 2.06% |

The Level III program has also been used, with the default model, using the same input parameters.
The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 71.9 | 0.0324 | 0.000287 |
| % in water | 3.18 | 45.9 | 0.0674 |
| % in sediment | 3.74 | 54 | 0.0792 |
| % in soil | 21.2 | 0.00954 | 99.9 |

The results reflect that the ultimate fate of 1-decanol is dependent on its route of release into the environment.
1-Decanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.
In water, the adsorption coefficient of 1-decanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (5)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 4.57 was used in the TGD calculation methods.

**Result:**
TGD Hydrophobics method: Koc = 6330
TGD Non-hydrophobics method: Koc = 2490
TGD Alcohols method: Koc = 190

SRC PCKOCWIN method: Koc = 96
**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (4)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 2 mg/l related to Test substance
5 mg/l related to Test substance
**Contact time:** 30 day(s)
**Degradation:** = 88 % after 30 day(s)
**Result:** readily biodegradable
**Kinetic:** 5 day(s) =
15 day(s) = 74 %
30 day(s) = 88 %
**Control Subst.:** other: Dodecylsulfate

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1983
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. The dispersing agent was nonylphenol ethoxylate additionally propoxylated with 5 propyleneoxide units (NP 9,5 EO 5PO). The ratio of test substance to emulsifier was 1:1. The final concentrations of test substance were 2 and 5 mg/l.

The following validity criteria were met:
(1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and
(4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l at the lower test concentration. At the higher test concentration, the
reported dissolved oxygen concentration was below 0.5 mg/l from Day 5 onwards.
**Result:** Kinetic of control substance:
5 days = 73%
15 days = 80%
30 days = 96%
The test substance (2 mg/l) attained >60% degradation within the 10 day window and can therefore be considered readily biodegradable. The values reported in the results
section are for the 2 mg/l concentration. The 5 mg/ltest concentration had insufficient residual dissolved oxygen content. The following results were given, 5 day >53%; 15 day

>60%; 30 day >60%.
**Test condition:** Concentration of inoculum: 1 ml/l (about 10E3 - 10E5 cells/ml)
Test volume: 292.8 - 294.5 ml
Temperature: 20 C
pH: not reported
**Reliability:** (2) valid with restrictions
The test was not conducted to GLP and did not meet one of the validity criteria for the test at the higher test concentration.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (72)

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 50 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 77 % after 30 day(s)
**Result:** readily biodegradable

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Biological Oxygen Demand Test for Insoluble Substances (BODIS). This method is based on the Closed Bottle Test (OECD test method 301D) and the RDA-Blok Test.
The test medium is inoculated with a mixed bacterial inoculum. After addition of a predetermined amount of test chemical (50 mg COD/l) the test vessels containing a known volume of aqueous test mixture (2/3) and air (1/3) are shaken continuously to assure steady state oxygen partitioning between liquid and gas phase. The degradation is followed by weekly measurements of the BOD in the aqueous phase during a 28-day period.
**Remark:** This information is from a summary of the full report. The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. No information is provided regarding the validity criteria.
**Result:** 15 days = 55%
30 days = 77%
Report states Decanol is readily biodegradable, however insufficient information is provided to interpret the 10-d window acceptability criterion.
**Reliability:** (4) not assignable
Summary report only available. There is insufficient information reported to assess the validity of this test.
05-OCT-2005 (43)

**Type:** aerobic
**Inoculum:** other: no details provided on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 54 % after 31 day(s)
**Result:** inherently biodegradable
**Kinetic:** 4 day(s) = 32 %
10 day(s) = 46 %

17 day(s) = 51 %
24 day(s) = 53 %
31 day(s) = 54 %

**Control Subst.:** other: Sodium benzoate

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** No information is provided regarding the validity criteria.
**Result:**
The test substance attained <60% degradation during the test period and therefore cannot be considered readily biodegradable.
Kinetic of control substance: 4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
**Reliability:** (4) not assignable
The information reported is insufficient to assess the validity of this study.
05-OCT-2005 (101)

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 10 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 29 day(s)
**Degradation:** = 29 % after 29 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 5 day(s) = 18 %
15 day(s) = 26 %
29 day(s) = 29 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A five-day bacterial inhibition test was performed under the conditions of the Closed Bottle Test. In a subsequent Modified Sturm Test, the test material was added to two vessels containing mineral salts medium and activated sludge to give a nominal test concentration of 10 mgC/L. Control vessels comprised two containing inoculated mineral salts medium alone and one containing inoculated mineral salts plus sodium benzoate (10 mgC/L). Test and control vessels

were aerated for 29 days with air that had been treated to remove CO2.

**Remark:** Cumulative CO2 production in the controls after 29 days (77.8 and 80.1 mgCO2) was within the acceptable range for this assay system (recommended maximum = 120 mgCO2 for a three litre culture). The reference compound reached the pass level within 14 days and the parallel assays did not differ by more than 20%. No information is given on total inorganic carbon levels at the start of the test.

**Result:**

The test substance attained <60% degradation during the test period therefore it cannot be considered readily biodegradable.
Kinetic of control substance: 5 days = 61%
15 days = 82%
29 days = 89%

**Test condition:** Total solids concentration of inoculum: 30 mg/l
Temperature: 21.2 - 23.9°C
pH: 7.4 - 7.6

**Reliability:** (2) valid with restrictions
Guideline study although some validation data not reported.

09-SEP-2005 (47)

**Type:** aerobic
**Inoculum:** other: municipal sewage treatment plant effluent
**Concentration:** 2 mg/l related to Test substance
**Degradation:** = 86 % after 30 day(s)
**Result:** readily biodegradable

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Values corrected for control (emulsifier alone). parameter: % BOD/COD
**Source:** Henkel KGaA Duesseldorf
**Test condition:** Biologically hard Nonylphenol 10EO/5PO used as emulsifier.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

10-JAN-2005 (34)

**Type:** aerobic
**Inoculum:** domestic sewage, adapted
**Degradation:** = 36.3 % after 5 day(s)

**Method:** other: 5 day BOD according to "Standard Methods for the
**Year:** 1980
**Test substance:** as prescribed by 1.1 - 1.4
**Source:** Henkel KGaA Duesseldorf
**Test condition:** 21 +/- 3 degr. C, parameter: BOD5 [mmole/mmole substrate]/ BOD theoretical. Microbial culture from domestic sewage adapted to test substance prior to test.

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
10-JAN-2005 (8)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 2 mg/l
**Degradation:** = 66 - 80 % after 30 day(s)
**Result:** readily biodegradable

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Original experimental data: erheblich getrübte Stammlsg. Lösungsvermittler eingesetzt ungenügender Restsauerstoff in der höheren Prüfkonzentration..
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 2 mg/l referring to Active Substance: 86% with parameter % BSB/CSB
#2: 5 mg/l referring to Active Substance: 60% with parameter % BSB/CSB
**Test substance:** Analogy; data taken from CASRN 112-30-1 <1-Decanol>, Active Matter = 100 %.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (36) (37) (39)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**GLP:** no data
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.
BOD was determined by measurement of dissolved oxygen concentrations in the test vessels at the start and end of the test period.
**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.
**Result:** 36.3% degradation after 5 days (% ThOD)
**Test substance:** As prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
Non-guideline study.

17-OCT-2005 (95)

**Method:** other: Assessed using methods based on OECD Guideline 301D (Closed Bottle Test) and Procedure C.4-E of the Annex to Directive 92/69/EEC
**GLP:** no data
**Year:**
**Method:** Triplicate mixtures containing the test substance at nominal concentrations of 5 mg/L and 2.5 mg/L in mineral salts medium inoculated with final effluent from a sewage treatment plant were incubated for five days. The COD of the test material was determined by oxidation with an acid-dichromate mixture using a semi-micro procedure, in which Cr(VI) is reduced to Cr (III).
**Result:** The mean BOD was 0.27 gO2/g. The mean COD was 2.67 gO2/g.
The BOD:COD ratio ranged from 5 to 15%.
The mean 5 day BOD of Kalchol 1095 was 10% of its COD.
**Test condition:** Concentration of inoculum: 5 ml/l
Test volume: not reported
Temperature: 20.4-20.7 C
pH: 7.1-7.6
**Test substance:** As prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
17-OCT-2005 (48)

## 3.7 Bioaccumulation

**BCF:** = 1530

**Method:** other: calculated (Veith et al, 1979)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.
The measured log Kow value of 4.57 was used in the calculation.
**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.
The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (4)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 2.3
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Both Veith et al. citations (1983a and 1983b) have the same authors and report the same data. It is likely this is the same study as reported in Brooke et al 1994. Veith reports results for juveniles and Brooke reports results for fry. The publication indicates that test concentrations were monitored daily, however, the results are not provided.

**Result:**
RESULTS: EXPOSED
LC50 = 2.3 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

**Test condition:**
TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5

Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test, although analysis results were not provided.

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (19) (98) (99)

**Type:** static
**Species:** other: Salmo gairdneri (rainbow trout) and Lepomis macrochirus (bluegill)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** > 4.2 - 5.6
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test compound was added to each jar in a solution of acetone. A control which contained the greatest amount of acetone introduced into any test was conducted. Ten fish were exposed to a range of concentrations (2.4-10 mg/L for Rainbow trout and 3.2-10 mg/l for bluegill) and a control. Static bioassays were conducted at 21 C for the bluegill and at 12 C for the rainbow trout, both at a pH of 7.1. The bluegill had a mean weight and length of 1.0 g and 36 mm and the rainbow trout weighed 1.2 g and was 56 mm in length.
**Result:** The 96-h LC50 was 5.05 for bluegill and >4.2 - < 5.6 for rainbow trout. The highest concentrations at which there was no discernible effect (NOEC) during the 96-h bioassay was 3.2 mg/l for the bluegill and 2.4 mg/l for the rainbow trout. Prior to death, fish generally became dark and lethargic and lost equilibrium.

No mortalities were observed in any of the control groups.

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
17-OCT-2005 (24)

**Type:** static
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = 1
**LC50:** = 5.7
**Limit Test:** no

**Method:** other
**Year:** 1996
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** In this preliminary toxicity screen, groups of five fish were exposed to the test substance at nominal concentrations of 0.1, 0.32, 1, 3.2, 10, 32, and 100 mg/L. Control groups of fish were placed into dilution water alone or dilution water containing HCO-40 at the same level as in the test medium at the highest concentration. Observations of the fish were made at 24-hour intervals.
**Result:** Sublethal, treatment-related effects were noted at 3.2 mg/L and higher concentrations and included hyperventilation, darkened pigmentation, lethargy and loss of coordination. All fish were adversely affected within 15 minutes of exposure.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
19-JUL-2005 (49)

**Type:** static
**Species:** Alburnus alburnus (Fish, estuary)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 7.2
**Limit Test:** no

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available
19-JUL-2005 (15) (62)

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC0:** = 5.6
**LC50:** = 8.4
**LC100:** = 11
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.

**Remark:** This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. Mortalities are recorded at least at 24 hour intervals.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
19-JUL-2005 (44)

**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** = .4 - 1
**LC50:** = .6 - 3.2
**LC100:** = .8 - 10

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available.
19-JUL-2005 (100)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 1.9 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (3)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = .3
**EC50:** = 2.9
**EC100:** = 29
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11).
This method corresponds to the OECD Guideline 202, part 1.
**Remark:** Static exposures. Endpoint was immobilization. This information is from a 1 page summary of the full report which is not available but an OECD standard method was used. 20 animals per concentration.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
19-JUL-2005 (42)

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 3.1
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available
19-JUL-2005 (15) (62)

**Species:** Daphnia magna (Crustacea)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 4.4

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.
**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available, data obtained from secondary literature
19-JUL-2005 (92)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = 2.8
**LC50 :** = 6.5
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1976
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Static bioassays were conducted using replicate vessels, which were maintained at 22 C. Five daphnids (less than 24 hours old) were randomly assigned to each test vessel within 30 minutes after ALFOL 10 was added for a total of 15 Daphnia per concentration. Five concentrations plus control were tested.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
05-OCT-2005 (25)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 11
**Limit Test:** no

**Method:** other
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Daphnids were 24 hours old to begin the test. Test medium was tap water free from chlorine, saturated with oxygen, hardness of 16, pH = 7.6 - 7.7, and temperature of 20-22 C.
**Reliability:** (4) not assignable
20-OCT-2005 (18)

**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 8.8
**EC50:** = 16
**EC100:** = 25

**Method:** other: static test

**Method:** Test condition: 20-22 degr. C, pH 7.6-7.7, parameter: mobility, no aeration, stock solution of test substance in water until optically clear.
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000

CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.

20-OCT-2005

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 2.1 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

21-DEC-2005 (3)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. 1 - 10

**Method:** other: read-across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 25

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
**Reliability:** (3) invalid
09-SEP-2005 (33)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = 10000

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of waste water on the oxygen consumption of Pseudomonas putida (L 27); DIN 38412 part 27.
The oxygen consumption rate of a bacterial suspension fed glucose as nutrient base is measured after a contact time of 30 minutes. The oxygen consumption rate of the same bacterial suspension in the presence of various concentrations of a test substance under otherwise identical conditions is also measured.
**Remark:** This information is from a summary of the full report.
The solubility of Decanol is about 37 mg/l, therefore the EC50 was not achieved at the solubility limit.
**Reliability:** (2) valid with restrictions
Not key study: Other studies tested closer to the limit of solubility are available
19-JUL-2005 (41)

**Species:** Bacillus subtilis (Bacteria)
**Unit:** mmol/l **Analytical monitoring:**
**EC50:** = .3

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 0.3 mmol/l = 47.5 mg/l
Parameter: inhibition of initial germination rate at 37 degr. C in phosphate buffer measured as reduction in absorbance at 650 nm pH 7.2.
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** Methanol as solvent (in concentrations not exceeding its minimum inhibitory conc. of 0.2 M).
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (105)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** 10000

**Method:** other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Original experimental data: LC0/EC0 entspricht der höchsten Prüfkonzentration.
Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (35) (38)

**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC50:** 8.83

**Method:** other: static test
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 95% confidence limits: 7.7 - 10.13 mg/l
cell growth photometrically determined (540 nm).
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (77)

**Species:** other bacteria: mixed microbial culture
**Exposure period:** 75 minute(s)
**Unit:** mol/l **Analytical monitoring:**

**EC50:** = .0028

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 0.0028 mol/l = 443 mg/l
Parameter: Oxygen consumption at 30 degr. C measured manometrically.

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

**Test condition:** Origin of microbial culture not specified. Culture adapted to growth on test substance prior to test.

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

11-OCT-2005 (94)

**Species:** other fungi: see remarks

**Method:** other: Test for inhibition of spore germination

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parameter: inhibition of spore germination
Species: no antifungal activity up to:

| | |
|---|---|
| Aspergillus niger | 100 mg/l (5 d; 28 degr. C; pH 5.6) |
| Trichoderma viride | * ( " ) |
| Trichophyton mentagrophytes | 100 mg/l ( " ) |
| Myrotecium verrucaria | 100 mg/l ( " ) |
| Candida albicans | 100 mg/l (20 h; 37 degr. C; pH 5.6) |
| Mucor mucedo | 100 mg/l ( " ) |

* antifungal activity at all concentrations tested (lowest tested concentration: 100 mg/l).

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

**Test condition:** petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l.

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

11-OCT-2005 (30)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

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## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)
**Unit:** µg/l **Analytical monitoring:** yes
**NOEC:** = 110 measured/nominal
**LOEC:** = 370 measured/nominal
**EC10 :** = 210 measured/nominal

**Method:** OECD Guide-line 211
**Year:** 2005
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 152, 411, 1110 and 3000 µg test item/L. Initial mean measured concentrations of freshly prepared test solutions were 1.6, 122, 351, 962, 2800 µg/L. Geometric means of mean measured initial and aged concentrations after 24 h hours were <LOQ, 23.3, 107, 367 and 1227 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was withdrawn. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with

sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: Daphnia magna STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each Daphnia magna was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The Daphnia magna were fed at each renewal with suspensions of unicellular green algae. The suspensions of Desmodesmus subspicatus (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to 15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 20.0 to 21.0°C, the light intensity was in the range 588 to 657 lux. The oxygen saturation never fell below 70 % (5.7 mg/L), and the mean pH was 9.4 to 9.5 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent Daphnia magna were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn Daphnia magna in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:
o Mortality (immobility) of parental generation Daphnia magna
o Age at first brood
o Total number of offspring per replicate
o Cumulative Number of live offspring per surviving female at the time of recording
o Intrinsic rate of increase, r
o Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by

liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-dodecanol-d25 as internal standard. The method was validated for the determination of the test item in Daphnia test medium in the concentration range of 1.0 - 100 µg/L

**Result:** SURVIVAL, GROWTH AND REPRODUCTION DATA

| Test item Nominal conc. (µg/L) | Survival (%) | Growth (length) Mean ± SD (mm) | Age at first brood Mean ± SD (days) |
|---|---|---|---|
| Control | 100 | 5.41 ± 0.22 | 8.9 ± 0.74 |
| 152 | 100 | 5.52 ± 0.19 | 9.2 ± 0.79 |
| 411 | 100 | 5.43 ± 0.21 | 9.0 ± 0.82 |
| 1110 | 100 | 5.26 ± 0.38 | 9.4 ± 0.97 |
| 3000 | 0 | n.d. | n.d. |

| Test item nominal conc. (µg/L) | Cumulative offspring per female Mean ± SD (#) | Intrinsic rate of increase r Mean ± SD (1/d) |
|---|---|---|
| Control | 68.1 ± 9.5 | 0.294 ± 0.017 |
| 152 | 68.0 ± 5.6 | 0.297 ± 0.018 |
| 411 | 62.9 ± 5.8 | 0.281 ± 0.011 |
| 1110 | 58.6 ± 7.7 * | 0.277 ± 0.024 * |
| 3000 | n.d. | n.d |

* significant difference to control according Williams-test (a = 0.05, one-sided smaller)

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 610 µg test item/L
EC20 = 1500 µg test item/L
LOEC = 960 µg test item/L
NOEC = 350 µg test item/L

Related to mean measured concentrations:
EC10 = 210 µg test item/L
EC20 = 670 µg test item/L
LOEC = 370 µg test item/L
NOEC = 110 µg test item/L

**Test substance:** C10 Fatty alcohol (1-Decanol)
CAS No. 112-30-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 21011
Purity: 99.5 % ± 0.5 %

**Reliability:** (1) valid without restriction
Guideline study conducted in accordance with GLP.

**Flag:** Critical study for SIDS endpoint

04-NOV-2005 (76)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

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### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**Species:** other: Anas platyrhynchos (duck) and Colinus virginianus (quail)
**Expos. period:** 5 day(s)
**Unit:** ppm
**LC50:** > 10000

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The animals were exposed to the appropriate dietary concentrations for five days, and then maintained on toxicant-free diet for an additional three-day observation period. Symptoms of toxicity and mortality were recorded daily throughout the study.
**Reliability:** (2) valid with restrictions
19-JUL-2005 (89) (90)

**Species:** other: Anas platyrhynchos (duck)
**Endpoint:** mortality
**Unit:** mg/kg bw
**LD50 :** > 4640

**Method:** other: The birds were given a single oral dose via capsule, then observed for 14 days.
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
19-JUL-2005 (68)

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP

may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (23)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:

n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.

No further information on other biotransformation pathways of these alcohols was provided.

**Source:** Kamil et al, 1953
Hayes Consultancy Service Bromley, Kent

**Test condition:** These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including C6-C18 alcohols included in this category, form glucuronic acid conjugates in the rabbit.

Groups of 3 Chinchilla rabbits, about 3 kg in weight, were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.

The results were reported as the amount of extra glucuronic acid excreted as a % of dose.

**Test substance:** n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol

**Conclusion:** All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

07-OCT-2004 (59)

**Result:** Distribution results were reported for lauryl alcohol (98% pure). 95% of the dose adminstered was recovered from the application site at 24 hours after dosing. 0.13% remained in the body while 0.10% was excreted in the urine and faeces. 2.61% was excreted in expired air as CO2. The ratio of the amount of compound excreted via expired air to the amount absorbed is the expiratory excretion rat. It was 91% for lauryl alcohol. The respiratory excretion rates for all the other alcohols investigated were >65% although all the actual data is not reported.

Absorption decreased with increasing carbon chain length. The absorption rate was investigated in different solvents (squalene, castor oil, triethyl citrate (TEC). The

percutaneous absorption rate of undiluted n-octanol was 50%, this was increased in squalene but decreased in castor oil or TEC. This was also reported with the other alcohols tested and the tendency was more pronounced at higher concentrations.

The degree of skin irritation was proportionally related to the degree of percutaneous absorption.

**Source:** Iwata et al, 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 3 hairless mice were used. The 1-C14 labelled test substances were applied to the dorsal skin using a plaster for a 24 hour period. Immediately following application of the test material each animal was placed in a container to measure expiratory excretion. At the end of the exposure period the treated area of skin was excised and dissolved using tissue solubiliser. The carcass was homogenised in a blender wwith sodium hydroxide. An aliquot of the homogenate was then dried and combusted for determination of radioactivity.

The effect of different solvents and concentration of the solvent was also investigated. The role of skin irritation in absorption of test substance was also examined.

**Test substance:** n-octyl alcohol; n-decyl alcohol, lauryl alcohol and cetyl alcohol all radiolabelled (1-C14) and >98% pure.

**Conclusion:** Following skin application of lauryl alcohol about 2.84 % of the administered dose was absorbed. Of this absorbed dose >90% was excreted in expired air (CO2). A similar trend was observed with the other alcohols tested. Absorption decreased with increasing carbon chain length and was affected by solvent and concentration.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

07-OCT-2004 (55)

**Remark:** 1-decanol is oxidised to decanal which is rapidly oxidised to decanoic acid. Decanoic acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Test substance:** As prescribed 1-decanol

**Reliability:** (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including 1-decanol.

25-NOV-2004 (103)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: COX-SD
**Sex:** male/female
**No. of Animals:** 60
**Vehicle:** other: Undiluted
**Doses:** 7.96, 12.62, 15.89, 20.00, 31.70 and 39.91 gm/kg

**Value:** = 19500 mg/kg bw

**Method:** other: contract laboratory procedure
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: between days 1 and 7.
- Number of deaths at each dose: 0/10, 2/10, 3/10, 7/10, 7/10, 10/10

CLINICAL SIGNS: Animals at each dose level displayed one or more of the following effects: hypoactivity, hypersalivation, diarrhea, malaise, unthriftness, hypersensitivity to touch, ventral alopecia (abdominal and perineal areas), generalized weakness, and emaciation. Twenty-five of the surviving animals returned to normal 2 to 10 days after dosage. Moderate to severe hypersensitivity to touch, emaciation and ventral alopecia persisted in the remaining six animals throughout the observation period. The three survivors at the 31.7 g/kg bw level experienced moderate to severe body weight loss.

NECROPSY FINDINGS: Twenty-one of the animals which succumbed showed one or more gross abnormalities: congestion of the kidneys, adrenals, liver, lungs, stomach and gastrointestinal tract, erosion of the mucosa of the translucent stomach, and linear and/or diffuse haemorrhages. Sacrificed animals revealed a proliferation of the mucosal tissues and depletion and visceral fatty tissue.

Gross necropsy of the animals sacrificed showed, in one, erosion, in twenty, proliferation of the mucosal tissues of the translucent stomach, and in three a depletion of the visceral fatty tissue. Necropsy findings in the remaining 11 animals did not reveal anything remarkable.

POTENTIAL TARGET ORGANS: Stomach, possible irritation of the mucosal lining.

SEX-SPECIFIC DIFFERENCES: None.
**Source:** Scientific Associates, Inc. 1977d
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: rats COX-SD
- Source: No data
- Weight at study initiation: 195 -274 g
- Controls: no
- Number/group: 5M+5F fasted

ADMINISTRATION:
- Doses: 7.96, 12.62, 15.89, 20.00, 31.70 and 39.91 gm/kg
- Doses per time period: single dose
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days.

EXAMINATIONS: The animals were observed several times on the day of dosing and daily thereafter. Gross necropsies were performed on all survivors and any animals which died during the observation period. Body weights of survivors were

recorded prior to sacrifice.

The LD50 was calculated using the method of Litchfield and Wilcoxon.

**Test substance:** Tradename Alfol 10

**Conclusion:** Rat oral LD50 of Alfol 10 is 19.5 g/kg (confidence limits (15.72-24.18), possible target organ, stomach mucosa.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

05-AUG-2005 (81)

**Type:** LD50
**Species:** rat
**Strain:** other: Holzman albiino
**Sex:** male/female
**No. of Animals:** 60
**Vehicle:** other: undiluted
**Doses:** 4.7, 6.63, 9.37, 13.24, 18.69, and 26.41 g/kg b.w.
**Value:** > 26410 mg/kg bw

**Method:** other: contract laboratory procedure
**Year:** 1965
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died.

CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed in any of the animals on the day of dosing. Diuresis lasted for less than 72-hours after dosage at the three lowest test levels. Diuresis, weakness, malaise, and bloody nasal discharge were evident at the three highest doses for less than a week. Posterior ventral hair loss was noted at the three highest levels after 6-days. The sacrificed animals showed normal weight gains with one exception. One animal at the highest dose level showed a loss of 5 grams.

NECROPSY FINDINGS: Gross necropsy of the sacrificed animals showed no abnormalities of the viscera. Loss of hair of the posterior ventral surface of the body was evident in all animals at the three highest levels.

POTENTIAL TARGET ORGANS: No obvious target organs.

SEX-SPECIFIC DIFFERENCES: Combined observations were reported so no conclusion could be drawn.

**Source:** Scientific Associates, Inc. 1965c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: rat
- Source: no data
- Weight at study initiation: 200-265 g
- Group size:5M+5F
- Controls: no

ADMINISTRATION:
- Doses: 4.7, 6.63, 9.37, 13.24, 18.69, and 26.41 g/kg b.w.
- Doses per time period: single

- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for clinical signs at regular intervals on the day of dosing and dialy thereafter. Following the 14 day observation perod all surviving animals were weighed, sacrificed and gross necropsies carried out. The LD50 was calculated by the Litchfield and Wilcoxon method.

**Test substance:** Tradename Alfol 10
**Conclusion:** Rat oral LD50 for Alfol 10 is >26.41 g/kg.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (78)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male
**No. of Animals:** 10
**Vehicle:** other: olive oil
**Doses:** 5 g/kg
**Value:** > 5000 mg/kg bw

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no deaths

CLINICAL SIGNS: There were no signs of toxicity.

POTENTIAL TARGET ORGANS: No conclusion could be drawn as there were no signs of toxicity and no pathological examination.

SEX-SPECIFIC DIFFERENCES: Males only tested.
**Source:** Potokar, 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS:
- Source: No data
- Age: adult
- Weight at study initiation: mean weight 170 g
- Controls: No

ADMINISTRATION:
- Doses: 5 g/kg
- Doses per time period: single dose
- Volume administered or concentration: 1ml/100g in olive oil.
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality.
**Test substance:** Tradename Lorol C10
**Conclusion:** The rat oral LD50 for Lorol C10 was >5 g/kg.

Also referred to in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
25-NOV-2004 (53) (71)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other: The rats were administered the test substance by gavage in a limit test and observed for a 14-day period.
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No adverse effects were observed during the observation period. The LD50 for male rats is >5000 mg/kg bw.
**Source:** Henkel KGaA 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat
- Source: no data
- Weight at study initiation: no data
- Group size: 10M fasted
- Controls: no

ADMINISTRATION:
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: observations of clinical signs and mortality.

Summary data only provided.
**Reliability:** (4) not assignable
Summary sheet only available, however would expect this to be a reasonable study as other Henkel reports are generally RL1 or 2.
05-AUG-2005 (40)

**Type:** LD50
**Species:** mouse
**Sex:** male/female
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Doses:** unspecified
**Value:** = 25000 mg/kg bw

**Method:** other
**Year:** 1963
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The mouse LD50 value for 1-decanol is 25 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain.

**Source:** Zaeva, 1963
Hayes Consultancy Service Bromley, Kent
**Test condition:** Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg), the actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination.
**Reliability:** (4) not assignable
Original document in Russian (translation available), experimental detail limited but result considered valid.
05-AUG-2005 (106)

**Type:** LD50
**Species:** mouse
**Strain:** no data
**Sex:** no data
**Value:** = 6500 mg/kg bw

**Test substance:** other TS: decyl alchol isomeric composition not specified

**Remark:** No other data available.
**Reliability:** (4) not assignable
Secondary reference. Original value reported in the Farm Chemicals Handbook 1991 which was not available for review and considered likely to be itself a secondary reference.
05-AUG-2005 (74)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Wistar
**Sex:** male
**No. of Animals:** 5
**Vehicle:** other: atmosphere generated with 55% ethanol
**Doses:** 10% of test substance in ethanol
**Exposure time:** 2 hour(s)

**Method:** other: in house protocol
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None of the animals died.

CLINICAL SIGNS: The rats showed no significant signs of intoxication other than falling asleep.

NECROPSY FINDINGS: Neither gross necrospy nor histopathological examination of the respiratory tract and lungs revealed any treament related effects.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: Males only tested.
**Source:** Potokar 1979
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Lorol 10
**Test condition:** TEST ORGANISMS: Rat (Wistar)

- Source: no data
- Weight at study initiation: average body weight 170 g
- Number of animals: 5 males
- Controls: 5 males receiving vehicle

ADMINISTRATION: inhalation
- Type of exposure: 2 hour exposure
- Concentrations: 10% test material in 55% ethanol, a control received ethanol only. The atmaospheric conentration was not monitored.
- Particle size: not reported
- Type or preparation of particles:

EXAMINATIONS: The animals were observed for 14 days, at the end of this period gross necropsies were performed and the lungs and respiratory tract removed for histopathological examination.

**Reliability:** (3) invalid
Insufficient study detail and non-standard atmosphere generation.

08-OCT-2004 (71)

**Type:** LC50
**Species:** rat
**Strain:** other: COX-CD
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: atmosphere generated as a mist
**Doses:** 71 mg/l
**Exposure time:** 1 hour(s)
**Value:** > 71 mg/l

**Method:** other: contract laboratory protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All rats survived the 1 hour exposure and subsequent 14 day observation period.

CLINICAL SIGNS: During exposure, all animals displayed hypoactivity and/or ataxia, salivation, and gasping. At the 24 hour period, all animals showed reddened encrustation about the eyes, nose and mouth and a roughened coat. All animals appeared normal within 96 hours following exposure. Final bodyweight records showed weight gains within the expected limits.

NECROPSY FINDINGS: Gross necropsy showed slight to moderate pulmonary congestion in all animals and adrenal congestion in 2 animals.

POTENTIAL TARGET ORGANS: The lungs were affected in all rats.

SEX-SPECIFIC DIFFERENCES:

**Source:** Scientific Associates, Inc. 1977a
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Alfol 10
**Conclusion:** The rat 1 hour LC50 for Alfol 10 (mist) was >71 mg/l. Signs of

intoxication during exposure included lethargy,and/or ataxia, salivation and gasping. Gross necropsy revealed congestion of the lungs in all animals.

**Test condition:** TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 216-253g
- Number of animals: 5m+5F
- Controls: none

ADMINISTRATION: 1 hour, inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a mist, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 71 mg/l for 1 hour (not monitored)
- Particle size: Droplet size not reported
- Type or preparation of particles: The mist was generated using a nebuliser.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (80)

**Type:** LC50
**Species:** mouse
**Strain:** no data
**Sex:** no data
**Exposure time:** 2 hour(s)
**Value:** = 4 mg/l

**Method:** other
**Year:** 1961
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of unobtainable Russian publication also reported in Iuclid 2000 and Patty 2001 (LC50 525 ppm). The only additional data available are confidence limits for the reported LC50 4 mg/l (+- 0.2)
**Reliability:** (4) not assignable
Secondary reference.
08-OCT-2004 (52) (53) (70)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: Undiluted alcohol spread over skin
**Doses:** 1, 2 and 4 g/kg
**Value:** = 2000 - 4000 mg/kg bw

**Method:** other: contract laboratory protocol
**Year:** 1976

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All deaths occurred within 3 days of exposure.
- Number of deaths at each dose: Intact skin 0/2, 0/4 and 2/2, abraded skin 0/2, 2/4 and 2/2.

LD50(s): Intact skin: 2-4 g/kg; Abraded skin: 2 g/kg; combined intact and abraded 2-4 g/kg. A visual assessment of test site suggested that >75% of the dose was absorbed at each dose level.

APPLICATION SITE: At the end of the exposure period all animals showed slight to moderate erythema and slight to marked oedema particularly of the ventral skin and particularly in animals with abraded skin. In all survivors, slight to severe drying and desquamation, wrinkling and coreaceousness of limited areas an multiple scattered pustular eruptions later occured persisting throughout the 14 day observation period.

CLINICAL SIGNS: Generalised weakness and inactivity in most animals following exposure. Survivors appeared normal at 72 hours post exposure. These signs persisted and/or intensified in animals which eventually died. Final body weights of surviving animals showed slight to moderate loss loss in 3 animals, remained constant in 1 animal, and showed slight to moderate gain in 6 animals.

NECROPSY FINDINGS: Dermal irritation as described above. Blanching, erosion and multiple focal haemorrhages of the gastric mucosa, haematuria and an accumulation of clear, viscous fluid within the peritoneal cavity were observed internally in animals which died prematurely.

Rabbits surviving to 14 days all showed moderate to severe desquamation with multiple interspersed scars at the application site (some 2-3 cm in diameter). Internally there was a slight accumulation of clear viscous fluid in the peritoneal cavity. There was blanching and/or focal haemorrhages and a granular texture to the gastric mucosa.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

**Source:** Scientific Associates, Inc. 1976b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.4 - 2.9 kg
- Group size: low dose and high dose 2M+2F and mid dose 4M+4F half with intact skin the others with abraded skin.
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the

animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 1, 2 and 4 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

**Test substance:** Tradename Alfol 10

**Conclusion:** The rabbit dermal LD50 for Alfol 10 was between 2000 and 4000 mg/kg (24 hour occlusive exposure). Dermal irritation was observed at the application site 24 hours after administration of the test material and persisted throughout the observation period. Generalised weakness and inactivity were commonly observed following the exposure period. Necropsy revealed blanching, erosion and focal haemorrhages in the gastric mucosa.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

05-AUG-2005 (79)

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male
**No. of Animals:** 6
**Vehicle:** other:
**Doses:** 1000 mg/kg
**Value:** > 1000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure period and 14 day observation period.

CLINICAL SIGNS: Confined to slight irritation of the skin reversible in 7 days. No signs of systemic toxicity.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified other than slight skin irritaton.

SEX-SPECIFIC DIFFERENCES: Males only tested.

**Source:** Potokar, 1979
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported

- Weight at study initiation: Not reported
- Group size: 6M
- Controls: No

ADMINISTRATION: 24 hour dermal occluded.
- Area covered: 10cm X 10cm
- Occlusion: gauze attached with plaster covered with plastic foil and then with elastic bandage.
- Vehicle: undiluted
- Doses: 1000 mg/kg
- Removal of test substance: Not reported.

EXAMINATIONS: 14 day observation period for mortality, signs of intoxication and local skin reaction.

**Test substance:** Tradename Lorol 10.
**Conclusion:** The rabbit dermal LD50 for Lorol C10 is >1000 mg/kg (24 hour occluded exposure). There were no signs of systemic toxicity only slight reversible skin irritation.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
08-OCT-2004 (71)

**Type:** LD50
**Species:** rabbit
**Value:** = 18.8 ml/kg bw

**Method:** other
**Year:** 1972
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of unobtainable Russian publication also reported in Iuclid 2000. No other information available.
**Reliability:** (4) not assignable
Secondary reference.
08-OCT-2004 (70)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**Result:** irritating

**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 1.7, 2.0, 2.0 (Group mean score 1.9)
- Oedema: All scores 0

REVERSIBILITY: At 7 days one animal only exhibited erythema. By 10 days all scores were 0 and the skin appeared normal.

OTHER EFFECTS: Loss of elasticity was reported at 48 and 72 hours after removal of the dressings. Control sites showed no evidence of skin irritation.

**Source:** Johnson 1996b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: out bred New Zealand white
- Sex: Female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.32-2.51 kg
- Number of animals: 3
- Controls: Untreated patches on same animals.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 3X2 cm
- Occlusion: semioccluded
- Vehicle: none
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 10 days
- Removal of test substance: warm water & paper tissues after 4 hours

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours after dressing removal and at 7 and 10 days.

**Test substance:** Tradename Kalcohl 1095
**Conclusion:** In this 4 hour semi-occlusive study Kalcohl 1095 (C12) would be considered a skin irritant under EU criteria with a mean 24+48+72 hour erythema score for 2 animals of >=2. Under GHS criteria this alcohol would be considered a mild irritant (category 3).
**Reliability:** (1) valid without restriction
Comparative study meeting generally accepted scientific principles.
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (56)

**Species:** rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 4

**Vehicle:** other: undiluted
**PDII:** 3.33
**Result:** moderately irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The in vivo data were generated in studies carried out since 1981 according to OECD Test guideline 404. The skin irritation data were collected from various sources to provide a reference data bank for validation of alternative skin testing methods. The data were obtained from tests normally using at least three rabbits evaluated at the same time involving applications of 0.5 g or 0.5 mL to the flank under semi-occlusive patches for 4 hours and in which observations were made at least 24, 48, and 72 hours after removal of the patch.

In the case of 1-decanol 4 rabbits were tested with undiluted 1-decanol of 98% purity. Observations were continued to 7 days.

**Result:** AVERAGE SCORE 24+48+72 hour
- Erythema: Individual 2.3; 2.3; 2.2; 1.8 Mean 2.15
- Oedema: Individual 2.0; 0.8; 1.0; 0.8 Mean 1.15

PII based on 24, 48 and 72 hour scores 3.33.

REVERSIBILITY: 7 days scores
- Erythema: Individual 1; 1; 2; 2 Mean 1.5
- Oedema: Individual 0; 0; 0.5; 0.5 Mean 0.25

OTHER EFFECTS: Desquamation was observed at all test sites at 7 days, this was described as marked in one animal.

**Source:** Bagley 1996.
Hayes Consultancy Service Bromley, Kent

**Conclusion:** Based on individual mean 24+48+72 hour scores of 2.3 for erythema in 2 of the 4 test animals plus persistence of the response to 7 days with desquamation in all animals it is considered that 1-decanol is irritating (Category 2) to the skin according to the GHS system and irritant according to EU criteria based on a group mean 24+48+72 hour score of 2.15 for erythema.

**Reliability:** (1) valid without restriction
Compilation of data conducted to OECD guidelines, reported in summary by Bagley, 1996 however full results available in ECETOC Technical Report No. 66, 1995.

**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (9) (26)

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Occlusive
**Exposure Time:** 8 hour(s)
**No. of Animals:** 5
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** other

**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No individual scores are given. The test material is reported as producing slight irritation which is reversible over the 14 day observation period. A score of 2,2 is reported but it is not clear exactly what this refers to.
**Source:** Potokar, 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS:
- Strain: Albino rabbits
- Sex: Male
- Age: Adult
- Number of animals: 5

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: Not reported
- Occlusion: Yes
- Vehicle: None
- Exposure period: 8 hours
- Postexposure period: 14 days
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: immediately after removal of patch then at 24 hours, observed until 14 days.

**Test substance:** Tradename Lorol 10.
**Conclusion:** Based on the limited data available it is considered that Lorol 10 is slightly irritating to the skin but unlikely to be a skin irritant under GHS or EU criteria.
**Reliability:** (4) not assignable
Documentation limited and insufficient for assessment but study appears a reasonably conducted standard Draize test.
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (71)

**Species:** other: rabbit, guinea pig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: vaseline

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** other TS: even C6-22 alcohols

**Result:** The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In all cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with

hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings (where available) together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

**Reliability:** (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.

05-AUG-2005 (53) (58)

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Occlusive
**Exposure Time:** 6 day(s)
**No. of Animals:** 5

**Vehicle:** other: undiluted
**Result:** highly irritating

**Method:** other: repeated skin application
**Year:** 1963
**GLP:** no
**Test substance:** other TS: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

**Result:** The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol.
**Source:** Zaeva, 1963 reported in BIBRA, 1995. Clayton and Clayton, 1994.
Hayes Consultancy Service Bromley, Kent
**Test condition:** Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental detaols were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol.
**Conclusion:** Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit skin for 6 consecutive days resulted in marked irritation with eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol.
**Reliability:** (2) valid with restrictions
Non-standard test with limited documentation.
08-OCT-2004 (16) (21) (106)

**Remark:** Report of a Czech publication, 1986. Very limited data, a 24 hour application of 20 mg test substance to the skin caused moderate irritation. No further details available.
**Test substance:** Decyl alcohol isomeric content not reported
**Reliability:** (4) not assignable
Secondary reference, original unavailable.
05-AUG-2005 (74)

**Species:** human
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 30
**Result:** not irritating

**Method:** other: human 4-hr patch test
**Year:** 1998
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Decanol produced a minimal response on human skin equivalent to that produced by water.
**Source:** Robinson et al, 1998
**Test condition:** O.2 ml undiluted decanol was applied to the skin of human

volunteers for up to 4 hours using a 25mm Hill Top chamber held in place with adhesive tape. The test site was scored on a 4 point scale. Once a positive response was observed in a given subject there was no further exposure to the material. A the end of the exposure excess material at the test site was removed using a damp towel. Sodium dodecyl sulphate was used as a positive control.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

05-AUG-2005 (73)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** moderately irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores 2, 1. 0.7 (group mean score 1.23)
- Iris: individual scores 0.7, 0.3, 0.7 (group mean score 0.56)
- Conjunctivae (Redness): 2.7, 1.3. 1.3 (group mean score 1.77)
- Conjunctivae (Chemosis): individual scores 1.3, 0.3, 0.3 (group mean score 0.63)

DESCRIPTION OF LESIONS: Slight or moderate conjunctivitis, very slight or slight corneal opacity and iritis were seen in all animals during the first 48 hours following instillation. On Day 4, all animals still showed slight conjunctivitis and one showed a small area of slight corneal opacity.

REVERSIBILITY: Slight conjunctivitis persisted in one rabbit to Day 8 and in another to Day 15. All scores 0 by day 22.

OTHER EFFECTS: Instillation of the test material caused a very slight initial pain response.

**Source:** Johnson 1996e
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: 5 months
- Weight at study initiation: 2.63 - 2.99 kg
- Number of animals: 3
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 22 days

EXAMINATIONS
- Scoring system: As prescribed in OECD test method.
- Observation period: 22 days
- Tool used to assess score: Ophthalmoscope or pencil beam torch. Fluorescein used from 24 hours onward as required to aid corneal examination.

**Test substance:** Tradename Kalcohl 1095
**Conclusion:** Kalcol 1095 is not an eye irritant according to EU criteria. Using GHS criteria Kalcol 1095 is an irritant category 2A based on scores for corneal opacity >= 1 in 2 rabbits and persistence >7 and <22 days.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (57)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** 1 other: drop
**Comment:** no data
**No. of Animals:** 5
**Vehicle:** none

**Method:** other: non standard
**Year:** 1963
**GLP:** no
**Test substance:** other TS: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

**Method:** One drop of undiluted material was instilled into the eye of 5 rabbits. No further experimental details are reported.
**Result:** All the alcohols studied caused redness and swelling of the mucous membranes of the eye. These disappeared almost completely within 4-5 hours. The most marked changes were observed with n-hexanol and are described as suppurative conjunctivitis and cloudiness of the cornea. There is no information given on the reversibility of these changes. The results suggest that except for 1-hexanol the alcohols tested are at most slightly irritating to the eye. With no information on the reversibility of effects over time no meaningful conclusion can be drawn about the degree of eye irritation caused by 1-hexanol in this study.
**Source:** Zaeva, 1963
Hayes Consultancy Service Bromley, Kent
**Reliability:** (3) invalid
08-OCT-2004 (16) (21) (106)

**Remark:** Secondary report from unobtainable Russian language reference. Corneal injury was reported following instillation of decanol into the eyes of rabbits. No further details available.
**Reliability:** (4) not assignable
Secondary reference.
26-OCT-2004 (70)

**Remark:** Secondary report from unobtainable Russian reference. 500 mg Decanol applied to the rabbit eye produced mild irritation.
**Reliability:** (4) not assignable
Secondary reference, original unavailable.
08-OCT-2004 (74)

## 5.3 Sensitization

**Type:** other: modified Draize test
**Species:** other: inbred Hartley albino guinea pigs
**Concentration 1st:** Induction 1.9 % intracutaneous
**2nd:** Challenge 10 % open epicutaneous
**3rd:** Challenge .75 % intracutaneous
**No. of Animals:** 10
**Vehicle:** no data

**Method:** other: modified Draize test
**Year:** 1978
**GLP:** no data
**Test substance:** other TS: decanol (random sample from commercial batch)

**Result:** RESULTS OF PILOT STUDY: 1.9%, 0.75% and 10% solutions were chosen for the intradermal induction, intradermal challenge and topical challenge respectively.

RESULTS OF TEST
- Sensitization reaction: No sensitisation following the original induction procedure. Individual animal data not reported. Sensitisation is reported after a second induction series however the actual number of animals responding is not reported. This suggests that the sample of decanol tested is at most a weak sensitiser. The authors note that they frequently find that weak sensitisers identifed by this repeated induction procedure do not induce sensitization in their guinea pig test when tested as an ingredient of perfume formulations. They also state that decanol did not produce sensitisation in the human maximisation test.
- Clinical signs: None
- Rechallenge: Sensitisation observed on challenge and/or rechallenge following a second induction procedure.

**Source:** Sharp, 1978
**Test condition:** TEST ANIMAL Guinea pig
- Strain: Hartley
- Sex: not reported
- Source: not reported
- Weight at study initiation: ca 350 g
- Number of animals: 10
- Controls: only at rechallenge

ADMINISTRATION/EXPOSURE
- Study type: Non-adjuvant
- Preparation of test substance for induction: not reported, 0.1 ml of the test solution was administered.
- Induction schedule: 4 intradermal injections at one time point over the 2 auxillary and 2 inguinal lymph nodes.
- Concentrations used for induction: Based on a primary irritation screen the concentration used was 2.5 times the

injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema).
- Challenge schedule: 14 days after induction each animal received an intradermal injection in one flank and a topical application on the other.
- Concentrations used for challenge: 0.1% intradermally and 10% topically
- Rechallenge: yes 7 days later if positive. If negative the induction procedure was repeated with subsequent challenge and rechallenge as appropriate, this time with controls at rechallenge.
- Positive control: not reported

EXAMINATIONS
- Grading system: A colour matching lighting unit was used to examine the skin reactions. Each injection reaction was scored based on size, erythema and oedema and considered positive if the total score was greater than the total average of the control scores. Application reactions were scored on a scale of 0 to +++ and considered positive if individual reactions were => + and there was no erythema in the controls.

- Pilot study: A preliminary irritation study was undertaken to determine the injection challenge concentration (the concentration giving slight barely perceptible irritation with no oedema) and the application challenge concentration (the highest concentration producing no irritation).

**Conclusion:** In this non-adjuvant procedure (modified Draize) decanol produced a weak sensitisation reaction in guinea pigs only after two sets of induction injections and following topical and/or intradermal challenge. The authors note that they frequently find that weak sensitisers identifed by this procedure do not induce sensitization in their guinea pig test when tested as an ingredient of perfume formulations. They also state that decanol did not produce sensitisation in the human maximisation test.

**Reliability:** (2) valid with restrictions
Reasonable reporting of a modified Draize test, result reporting limited. Test sample not characterised.

**Flag:** Critical study for SIDS endpoint

30-DEC-2005 (82)

**Type:** other: human maximization test
**Species:** human
**No. of Animals:** 25
**Vehicle:** petrolatum
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: Kligman human maximization test
**Year:** 1973
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This reference reports in summary unpublished data provided by Kligman 1972.
**Result:** Under the conditions of this test 1-decanol was not a human skin sensitiser.
**Source:** Opdyke, 1973

Hayes Consultancy Service Bromley, Kent
**Test condition:** This patch test was carried out using the maximization procedure described by Kligman, A.M. The identification of contact allergens by human assay. III The maximization test: A procedure for screening and rating contact allergens. J. Invest. Dermatol. 47:393-409, 1966. There are variations in this procedure but we have no information as to which variation was used. The exposure would have been a 48 hour occlusive exposure and sodium lauryl sulphate may have been used to promote the response. The only experimental detail given for 1-decanol was that a panel of 25 volunteers were tested at a concentration of 2% in petrolatum.
**Reliability:** (4) not assignable
Documentation insufficient for assessment.
25-NOV-2004 (53) (69)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** rat **Sex:** no data
**Strain:** other: not specified
**Route of administration:** inhalation
**Exposure period:** 2 hr/day
**Frequency of treatment:** 6 d/wk for 4.5 months
**Post exposure period:** none
**Doses:** Single exposure level between 0.18 and 0.35 mg/l.
**Control Group:** yes, concurrent no treatment

**Method:** other
**Year:** 1963
**GLP:** no
**Test substance:** other TS: 2-octanol, n-heptanol, n-decanol

**Result:** Minor changes in haematological parameters (decreased Hb & white cell count) were not of statistical significance. A reversible increase in the threshold of neuromuscular excitability was observed after 3.5 months exposure to n-heptanol(9.6(+-0.26) mA and 2-octanol 9.2(+-0.35 mA) compared to controls 8.2(+-0.25 mA), decanol treated animals were similar to controls. The behaviour of the exposed animals was comparable to that of controls as was body weight gain. There were no gross pathological changes. Minor histopathological changes (dystrophic) were reported in various organs including the liver, kidneys and myocardium. The incidence of these changes in treated and control animals was not clearly reported, the effects appeared more marked in animals exposed to n-heptanol and 2-octanol. With n-heptanol and 2-octanol there was some evidence of mild irritation of the respiratory tract. (The results for 2-octanol have been reported in summary by BIBRA 1995 and Patty 1994.)
**Source:** Zaeva, 1963 reported in BIBRA, 1995. Clayton and Clayton, 1994.

Hayes Consultancy Service Bromley, Kent
**Test condition:** Groups of 8 rats were exposed to a single dose level of either n-heptyl, n-octyl (2-octanol) or n-decyl alcohol for 2 hours/day, 6 days/week for 4.5 months. The actual dose level at which each alcohol was tested was not reported, the dose levels were reported as between 0.18 and 0.35 mg/l (33.8 -

56.3 ppm). There was a concurrent control group consisting of 8 untreated animals. The effect of these alcohols on the test animals was evaluated by clinical observations, body weight gain, neuromuscular response to electrical stimulation, effect on peripheral blood [Hb, RBC, WBC (plus differential WBC count)] together with macroscopic and histopathological examination of some organs.

**Reliability:** (3) invalid
Significant methodological deficiences and insufficient documentation for assessment.

25-NOV-2004 (17) (21) (106)

**Remark:** Secondary report of Russian language reference, 1988. This summary data reports effects in rats following repeated inhalational exposure to 180 mg/m3 decanol (isomers not specified), 4 hours/day for 137 days. Effects noted were degenerative changes to the brain and meninges, multiple effects on the liver and unspecified effects on the urinary system. Unspecified effects were reported on the sense organs following repeated inhalation exposure to 58 mg/m3 for 26 weeks.

From the same source information is provided of a rabbit inhalation study where 200 mg/m3, 2 hours/day for 30 days caused effects on the optic nerve together with corneal damage and an effect on true cholinesterase.

An additional secondary source for the rabbit study, reported by RTECS, is NTIS document PB 234-882, Scientific Literature Review of Aliphatic Primary Alcohols, Esters and Acids in Flavor Usage.

**Test substance:** Decanol (isomeric content not specified)
**Reliability:** (4) not assignable
Secondary reference, original not available.

14-SEP-2005 (74)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames test)
**System of testing:** Salmonella typhimurium strains TA98 and TA100
**Concentration:** 0.5 to 50 ug/plate
**Cytotoxic Concentration:** Slight thinning of background lawn at 50 ug/plate.
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: Ames
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
Preliminary study - Preliminary study without metabolic activation - At dose levels of 250 ug/plate and above there was an absence of revertant colonies with background lawn thin or absent. At 50 ug/plate there was slight thinning of background lawn with good population of revertant colonies. At 25 ug/ml there was no thinning of background lawn.

Main study - With and without metabolic activation: no increase in reverse mutation rate at any test concentration. All positive and negative controls showed an appropriate response.
PRECIPITATION CONCENTRATION: None reported.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: A slight thinning of the bacterial lawn was observed at 50 ug/plate.

**Source:** Huntingdon Life Sciences Ltd 1996l.

Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA98 and TA100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced.

ADMINISTRATION:
- Dosing: 0.5, 1.6, 1.8, 5 and 50 ug/plate. Dose selection was based on a preliminary toxicity screen with TA98 in which dose levels up to 5000 ug/plate were tested.
- Number of replicates: Duplicate
- Application: Pour plate, solvent DMSO.
- Positive and negative control groups and treatment: Negative controls DMSO and untreated bacterial control. Positive controls benzo[a]pyrene 5 ug/plate, sodium azide 2 ug/plate, 2-nitrofluorene 1 ug/plate.
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Not reported assume as for OECD 471

**Test substance:** Tradename Kalcohl 1095

**Conclusion:** The C10 alcohol Kalcohl 1095 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 50 ug/plate. There was evidence of cytotoxicity at the highest dose level (50 ug/plate).

**Reliability:** (2) valid with restrictions
Ames test no protocol specified but similar OECD 471 using only 2 tester strains. Criteria for evaluation not reported.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (50)

## 5.6 Genetic Toxicity 'in Vivo'

**Type:** Sister chromatid exchange assay
**Species:** Chinese hamster **Sex:** no data
**Route of admin.:** i.p.

**Method:** other: in vivo sister chromatid exchange assay
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no increase in sister chromatid exchange in the cells treated with 1-decanol alone, the level of SCE (2.8

+_0.3 SCE/cell) was comparable with controls (2.9 +-0.2 SCE/cell). When injected in the presence of NMU 1-decanol reduced the incidence of SCE seen with NMU alone

**Test condition:** 1-decanol prepared as an emulsion in saline was injected intraperitoneally into a single Chinese hamster aged between 12-13 weeks of age and weighing ca 30g at a dose level of 10(-3) moles/kg bw. 2 control animals received an injection of water. All animals received a subcutaneous implant of BrdU in the neck prior to treatment and injection of colchicine 2 hours before sacrifice at 24 hours. 50 cells from the control animals and 25 from the treated animals were scored for induction of SCE. The study was carried out as part of an investigation of the effects of n-alkanols on the induction of SCE by NMU and NMU acted as a positive control.

**Reliability:** (3) invalid
Significant methodological deficiencies, use of only one test animal limits the validity of this study. In the secondary publication by Tucker et al, 1993 this study is considered as inadequate or equivocal.

08-OCT-2004 (86) (91)

**Type:** Cytogenetic assay
**Species:** rat **Sex:** male
**Route of admin.:** other: intragastric
**Exposure period:** 48 hours
**Doses:** 1/5th LD50
**Result:** ambiguous

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:
600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 0.2 +-0.2
Cells with breakages %: controls 0.3 +-0.2; treated 1.8 +-0.5;
Cells with chromosome aberrations %: controls 0; treated 3.6 +-0.8.

**Source:** Barilyak, 1988
**Test condition:** TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage
- Vehicle: Homogenised emulsion
- Duration of test: 48 hours

- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Conclusion:** Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability:** (3) invalid
Significant methodological deficiences (see test conditions).

08-OCT-2004 (11)

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5-C24-34) are negative including a study for 1-decanol [Ames].

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions

The studies on which the conclusion for lack of genotoxic potential in vivo is based are either comparable to or guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (51) (84) (85) (97)

## 5.7 Carcinogenicity

**Species:** mouse **Sex:** female
**Strain:** Swiss
**Route of administration:** dermal
**Exposure period:** 60 weeks
**Frequency of treatment:** three times weekly
**Post exposure period:** none
**Doses:** 4 ug/mouse in cyclohexane
**Result:** ambiguous
**Control Group:** no

**Method:** other: skin tumour promotion study
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.

**Source:** Sice 1966.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane
- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)
- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Test substance:** Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol were investigated in this study. The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Conclusion:** In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999).

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

08-OCT-2004 (7) (53) (66) (67) (70) (83)

**Species:** mouse **Sex:** no data
**Strain:** other: Swiss albino ddY
**Route of administration:** i.p.
**Exposure period:** 5 days
**Frequency of treatment:** daily
**Post exposure period:** 24 days
**Doses:** Test 1: 2.5 or 10 mg/mouse/day. Test 2: 2, 4 or 8 mg/mouse/day 2.5 and 10 mg/mouse/day for C16 & 18 alcohols.
**Result:** negative
**Control Group:** yes

**Method:** other: determination of antitumour activity against Ehrlichs Ascites Tumour
**Year:** 1972
**GLP:** no
**Test substance:** other TS: other TS: Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** The C10, 12, and 14 alcohols exhibited toxicity to the mice, evidenced by severe diarrhoea and loss of body weight. The dose levels were reduced in the repeat test. The mean survival time for the untreated control group (Ascites implantation only) was 18.3 days in test1 and 14.4 days in test 2. All of the alkanols tested increased the survival time of mice

implanted with ascites tumour cells at one or more dose levels tested. Life span was prolonged by 124 - >194%.

**Source:** Ando et al, 1972
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS Mouse Swiss albino ddY implanted ip with ascites tumour cells.
- Age: 5 weeks
- Weight at study initiation: 20-23g
- Number of animals: 4 or 6/ treatment group, 20 controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 5 days starting 24 hours afeter implantation of the ascites tumour cells.
- Type of exposure: Intraperitoneal
- Post exposure period: 24 days
- Vehicle: Probably aqueous suspension using Tween 80.
- Concentration in vehicle: Not reported.
- Doses: Test 1: for all 5 alcohols tested dose levels were 2.5 and 10 mg/mouse. Test 2: C10, 12 and 14 alcohols were tested at 2, 4 and 8 mg/mouse, C16 and 18 alcohols were tested at 2.5 and 10 mg/mouse.

OBSERVATIONS
The mean survival time was recorded and compared to the untreated control group.

**Conclusion:** Treatment with C10 -18 alcohols extended the survival time of mice implanted intraperitoneally with Ehrlich ascites tumour cells.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint
08-OCT-2004 (1)

## 5.8.1 Toxicity to Fertility

**Remark:** Reproduction: The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C10 alcohol (1-decanol) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of effect on the reproductive potential is based are either comparable to

guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (84) (85) (97)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Species:** rat **Sex:** female
**Strain:** Sprague-Dawley
**Route of administration:** inhalation
**Exposure period:** 19 days
**Frequency of treatment:** 7-hours/day
**Duration of test:** 20 days
**Doses:** 100 mg/m3
**Control Group:** yes
**NOAEL Maternal Toxity:** > .1 mg/l
**NOAEL Teratogenicity:** > .1 mg/l

**Method:** other
**Year:** 1990
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL : 0.1 mg/l for maternal and foetal toxicity. No evidence of maternal toxicity, foetotxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5-10% of the nominal concentration of 0.1 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study. Actual dose achieved 0.1 mg/l.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: Comparable in treated and control groups. Mean resorptions/litter control 0.5, treated 0.5.
- Number of corpora lutea: Comparable between treated and control groups. Mean corpora lutea/litter control 14.9, treated 13.8.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Comparable between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Litter size (mean) control 13.5, treated 13,1.
- Sex ratio: No significant difference between treated and controls. Controls/litter (mean) male 6.6, female 6.9;

Treated/litter (mean) male 6.8, female 6.3.
- External, Soft tissue and Skeletal abnormalities: No treatment related effects.

**Source:** Nelson et al. 1990.
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
Groups of approximately 15 female pregnant Sprague-Dawley rats with a mean maternal weight of 281 g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose level: 0.1 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F.
- Control group: The treated animals were compared with pooled controls from 11 studies using the same protocol conducted over a 5 year period.
MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA. Foetal incidence data were analysed using the Variance Test for Homogeneity of the Binomial Distribution or ANOVA. The Kruskal-Wallis test was used if a non-parametric analysis was more appropriate.

**Conclusion:** The NOAEL for maternal toxicity, foetotoxicity and teratogenicity to rats following inhalation exposure to n-decanol during gestation (Gestation days 1-19) is 0.1 mg/l (the highest attainable concentration). There were no adverse effects on any of the maternal or foetal parameters investigated.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (46) (64) (65) (74)

**Species:** rat **Sex:** female
**Strain:** no data
**Route of administration:** other: intragastric
**Exposure period:** Gestation days 1-15

**Frequency of treatment:** daily
**Duration of test:** to gestation day 20
**Doses:** 1 ml of 40% aqueous suspension
**Control Group:** yes, concurrent vehicle

**Method:** other: non-standard
**Year:** 1991
**GLP:** no data
**Test substance:** no data

**Result:** NOAEL : Not established, the single dose level produced evidence of foetotoxcity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL: 400 mg/rat

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None reported
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Preimplantation loss: 15.1% (+- 3.5%) treated; 2.0% (+- 1%) controls.
- Number of resorptions: 17.8% (+- 4%) in treated rats); 4.4% (+- 1.4%) in controls.
- Number of corpora lutea: Comparable between treated and control groups.
- Body weight: Not reported
- Food/water consumption: Not reported
- Description, severity, time of onset and duration of clinical signs: Not reported
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.
- Other: placental weight was not significantly affect by treatment.

FOETAL DATA:
- Litter size and weights: Not reported only total mean foetal weights reported these were not significantly affected by exposure to decanol. Treated group foetal weight 2.36 g (+- 0.05) controls 2.25 g (+- 0.02).
- Sex ratio: Not reported.
- External, Soft tissue and Skeletal abnormalities: No externally visible developmental anomalies. Developmental effects on the internal organs and skeleton were observed in 4.8% (+- 1.2%) of foetuses exposed to decanol and 1.2% (+- 0.3%) of controls. These effects were not reported separately. The types of effect seen in the alcohols tested were hydrocephalus, hydronephrosis and retardation of ossification there was no indication of the frequency of these defects for each alcohol tested.
- Effect on Alcohol Dehydrogenase (ADH): Decanol reduced the ADH level in 20 day rats by 69.6%.

**Test condition:** TEST ORGANISMS: rat initial weight 160-180g

ADMINISTRATION / EXPOSURE
- Type of exposure: intragastric

- Duration of test/exposure: gd 1-15
- Control group and treatment: 1 ml/rat water, 20 controls
- Vehicle: water
- Concentration in vehicle: 40% suspension
- Total volume applied: 1 ml/rat
- Doses: 1 ml 40% aqueous suspension (400 mg/rat) to 10 rats.

MATING PROCEDURES: Sprem positive females

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Not reported
- Food & water consumption: Not reported.
- Clinical observations: No data
- Examination of uterine content: Gestation day 20, number of corpora lutea, implantations, resorption sites, placental weight and size and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights were recorded.

OTHER EXAMINATIONS: Measurement of alcohol dehydrogenase in the liver of foetuses between GD 16 and postnatal day 20.

STATISTICAL METHODS: Analysis of variance.

**Test substance:** Test substance described as decanol, no indication of purity or isomer content. Decanol was tested as part of a comparative study of C1-C10 alcohols.

**Conclusion:** This study suggests that decanol may induce foetotoxicity at a dose level of 400 mg/rat, how methodological deficiencies and inadequate reporting render this investigation of questionable validity.

**Reliability:** (3) invalid
Significant methodological deficiencies (small group size), analysis not conducted on a litter basis, no reporting of maternal status) coupled with insufficient documentation.

06-APR-2005 (10) (74)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: human skin irritation

**Result:** Hexanol and octanol gave responses significantly lower than the postive control and results were similar between laboratories. These alcohols were therefore not considered as skin irritants.

Decanol gave equivocal responses, an initial test gave a response just sufficient to classify as irritant. Subsequent testing by 3 other laboratories did not confirm this result.

**Source:** Griffiths et al, 1997
Hayes Consultancy Service Bromley, Kent

**Test condition:** These materials were tested as part of an interlaboratory evaluation of a human patch test for identification of skin irritation potential.

Groups of at least 30 volunteers were used for each evaluation at each location, at least 2 locations tested each product. The undiluted material (0.2 ml) was applied to the outer arm using a Hill Top chamber for a period usually of 4 hours. the reaction was assessed at 24, 48 and 72 hours after initiation of the exposure. SDS (sodium dodecyl sulphate) was used as a positive control. If the proportion of the test group reacting to the test material was significantly less that those reacting to the positive control the material was considered as not classifiable as a skin irritant.

**Test substance:** hexanol, octanol, decanol

**Reliability:** (2) valid with restrictions

05-AUG-2005 (31)

**Type:** other: human skin irritation

**Remark:** The purpose of this study was to introduce the chamber-scarification test designed for increased sensitivity for assessing the irritancy of materials. It should be noted that persons especially vulnerable to irritants were selected.

The materials were applied as a 25% solution in mineral oil. The skin is first scarified and the test material applied (0.1 ml) in a test chamber once daily for 3 days to groups of 5-10 volunteers. The skin was assessed 30 minutes after the end of the final exposure.

The degree of irritation was related to carbon chain length, the C10 and C12 alcohols giving a marked response while the C14 alcohol gave a moderate response, C16 slight and the oleyl alcohol gave a low response.

This work was presented at the 3rd conference on Cutaneous Toxicity, Washing DC, 1976 and published in the conference proceedings in Cutaneous Toxicity eds Drill & Lazar. This referred to by RTECS, 2004.

**Source:** Frosch & Kligman, 1976
Hayes Consultancy Service Bromley, Kent

**Test substance:** oleyl alchol, hexadecyl alcohol, tetradecyl alcohol, dodecyl alcohol, decyl alcohol

**Reliability:** (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment.

05-AUG-2005 (27) (74)

**Type:** other: allergic reaction in man

**Remark:** The authors report the results of patch testing with aliphatic alcohols in 1664 consecutive patients at a dermatological

clinic. Patch testing with decanol (5% in vaseline and olive oil) resulted in 15 positive reactions, patch testing with 10% in vaseline gave 22 positive reactions, an incidence of 0.9% and 1.3% respectively.

**Test substance:** Decanol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

25-NOV-2004 (45)

**Type:** other: aspiration

**Remark:** Aspiration of 0.2 ml 1-decanol to rats produced deaths in 9/9 rats immediately due to respiratory arrest.

**Conclusion:** In this screening test 1-decanol presents an aspiration hazard.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

25-NOV-2004 (29) (70)

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 112-42-5
**CAS No.** 112-42-5
**EINECS Name** undecan-1-ol
**EC No.** 203-970-5
**Molecular Formula** C11H24O

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
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**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** Paul-Baumann-Strasse, 1
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 20138 Milano
**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
02-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

02-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Undecanol
**Smiles Code:** OCCCCCCCCCCC
**Mol. Formula:** C11 H24 O1
**Mol. Weight:** 172.31

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-undecanol, CAS 112-42-5 are >80% linear.

The substance comprises >95% C11. Components of even and odd chain length, in the range C9-C14 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required

11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Undecanol (9CI) (CA INDEX NAME)
Undecyl alcohol (6CI, 8CI)
Hendecanoic alcohol
Hendecyl alcohol
n-Undecan-1-ol
n-Undecyl alcohol
Neodol 1
NSC 403667
Tip-Nip
Undecanol
Alcohol c-11 undecylic
Decyl carbinol
Undecan-1-ol
1-Hendecanol
1-Hydroxyundecane
1-Undecyl alcohol
Alchem 11

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-undecanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 150000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 7000 tonnes, consumption 13 000 tonnes (alcohols in range C6-11). This is publicly-available CEH data for Japan, for 2001.

21-DEC-2005 (8) (25) (33)

## 1.6.1 Labelling

**Remark:** Not required

11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.
21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification 2. ID No. 5632.
05-AUG-2005 (40)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-undecanol. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

02-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

02-AUG-2005

## 2.1 Melting Point

**Value:** = 14.3 degree C

**Method:** other: no information reported
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (24)

**Value:** = 11 - 19 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value taken from secondary literature
11-OCT-2005 (39)

## 2.2 Boiling Point

**Value:** = 245 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (24)

**Value:** = 131 degree C at 20 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value taken from secondary literature
11-OCT-2005 (39)

## 2.3 Density

**Value:** = .83

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (39)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0039 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (14)

**Value:** < .1 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (3) invalid
04-JAN-2005 (29)

**Value:** = .004 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
09-AUG-2005 (2)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 4.72

**Method:** other (measured)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original source not stated.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (1) (35)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 8 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (22)

**Solubility in:** Water
**Value:** = 8.3 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 8.3 mg/l at a loading rate of 100 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
09-SEP-2005 (2)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 16.78136E-12 cm3/molecule.sec
Half-life: 22.9 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

### 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
10-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:

Molecular weight 172.3
Data temperature 25 deg C
Log Kow 4.72
Water Solubility 8 mg/l
Vapour pressure 0.39 Pa
Melting point 14 deg C
half life in air 22.9 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 3.37% |
| Soil | 92.5% |
| Water | 1.99% |
| Fish | 5.22E-03% |
| Sediment | 2.06% |

The Level III program has also been used, with the default model, using the same input parameters.
The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 77.9 | 0.0414 | 0.000334 |
| % in water | 2.67 | 36.6 | 0.0458 |
| % in sediment | 4.64 | 63.4 | 0.0794 |
| % in soil | 14.8 | 0.00784 | 99.9 |

The results reflect that the ultimate fate of 1-undecanol is dependent on its route of release into the environment.
1-Undecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.
In water, the adsorption coefficient of 1-undecanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (5)

## 3.3.2 Distribution

**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 4.72 was used in the TGD

calculation methods.
**Result:** TGD Hydrophobics method: Koc = 8380
TGD Non-hydrophobics method: Koc = 2980
TGD Alcohols method: Koc = 220
SRC PCKOCWIN method: Koc = 180
**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (4)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.
**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.
**Result:** 27.6% degradation after 5 days (% ThOD)
**Test substance:** As prescribed in 1.1 - 1.4

**Reliability:** (2) valid with restrictions
11-OCT-2005 (34)

## 3.7 Bioaccumulation

**BCF:** = 2050

**Method:** other: calculated (Veith et al, 1979)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 4.72 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (4)

## 3.8 Additional Remarks

**-**

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 1.04
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
LC50 = 1.04 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported
The publication indicates that concentrations were monitored daily using analytical methods, however, no results are included.
**Source:** Veith et al. 1983a; Veith et al. 1983b.
**Test condition:** TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and

96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (37) (38)

**Type:** static
**Species:** Alburnus alburnus (Fish, estuary)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 4.6
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Source:** Bengtsson, 1984
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available
11-OCT-2005 (9) (23)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 1.7 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (3)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = .8 - 1.1
**Limit Test:** no

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two methods of test medium preparation were used, (1) C11 was dissolved in acetone, (2) Tween 80 was dissolved at 10% (by weight) of 96% ethyl alcohol and was shaken until an emulsion was obtained. This emulsion was added in 10% (by volume) to filtered brackish water and the mixture was shaken again for a couple of minutes until a new emulsion was obtained. It was considered that 100 ppm of this emulsion could be used as a solvent for the higher alcohols without any risk for the test animals.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Result:** RESULTS: EXPOSED
LC50 = 1.1 mg/l (Water/acetone)
LC50 = 0.8 mg/l (Water/Tween 80)
based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source:** Bengtsson, 1984
**Test condition:** TEST ORGANISMS
Strain: Nitocra spinipes
Supplier: Laboratory culture
Weight: not reported
Feeding: not reported
Pretreatment: not reported
Feeding during test: not fed during test
Control group: 2 control group (10 individualsin each)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle, solvent: concentration never exceeded 500 ul/l
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Natural Brackish water (filtered before use)
Aeration: No aeration
Alkalinity: 1.6 megv/l
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: Logarithmic series of at least 6 concentrations
Renewal of test solution: none

Exposure vessel type: 15ml standard laboratory test tubes
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 21 +/- 1 C
Dissolved oxygen: Not reported
pH mean: 7.9
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: lethality
SAMPLING: Mortality was recorded only after 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION:
not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (9) (23)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 1.8 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (3)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (6)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 12.5

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.

**Remark:** MIC = Minimal Inhibitory Concentration
**Source:** Hattori 1987.
**Reliability:** (3) invalid

11-OCT-2005 (18)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)
**Unit:** mg/l **Analytical monitoring:**
**NOEC:** = .044 - .17 calculated

**Method:** other: calculated (QSAR)
**Year:** 2005
**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

Structure-activity relationships have been developed based on these results. It is possible to apply these structure-activity relationships to estimate chronic toxicity endpoints where there are no reliable measured data.

Two QSAR relationships have been developed. It can be concluded that the NOEC for reproduction would be within the range of the two estimates.

**Result:** It can be estimated that chronic NOEC(reproduction) for Daphnia magna would lie in the range of 0.044 - 0.17 mg/l.

**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (7)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.
**Source:** de Wolf and Parkerton 1999.
**Reliability:** (2) valid with restrictions
30-OCT-2003 (15)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

**Remark:** Undecanol is oxidised to undecanal which is rapidly oxidised to undecanoic acid. Undecanoic acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.
**Test substance:** As prescribed Undecanol
**Reliability:** (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including undecanol.
25-NOV-2004 (41)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Doses:** 10,000 mg/kg
**Value:** > 10000 mg/kg bw

**Method:** other
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None

CLINICAL SIGNS: Reduced appetite and inactivity for 1-3 days post dosing.

NECROPSY FINDINGS: Unremarkable
**Source:** Younger, 1977
**Test condition:** TEST ORGANISMS: rats
- Source: no data
- Weight at study initiation: average 245 for male and female.
- Group size: 2M, 3F
- Controls: no

ADMINISTRATION: single dose oral
- Doses: 10,000 mg/kg
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Cinical signs, gross necropsy.
**Conclusion:** The rat oral LD50 for undecyl alcohol was >10 g/kg.
**Reliability:** (2) valid with restrictions
Screening test with basic information and result reporting. appears valid.

**Flag:** Critical study for SIDS endpoint
26-OCT-2004 (43)

**Type:** other: Range finding LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male
**Vehicle:** water
**Doses:** Administered in multiples of 10.
**Value:** = 3000 mg/kg bw

**Method:** other: Smyth & Carpenter, 1944
**Year:** 1944
**GLP:** no
**Test substance:** other TS: Reported as undecanol however no specific details of composition/purity in the publication

**Result:** The rat oral LD50 for undecanol was found to be 3 g/kg.
**Source:** Smyth and Carpenter 1944
Hayes Consultancy Service Bromley, Kent
**Test condition:** Rats weighing 90 to 120 g were given a single dose in water at an appropriate dose level derived by comparison with similar materials. Using multiples of 10 a further 6 rats were dosed a week later until two doses differing by a multiple of 10 are found one of which kills some or all animals within 14 day and the other kills some of no animals within this time period.
**Reliability:** (4) not assignable
Screening study limited result reporting but probably valid.
18-JUL-2005 (11) (16) (26) (32)

**Remark:** BIBRA report an oral rat LD50 value of >16 g/kg. This is an unpublished communication provided to BIBRA by Collins, 1988
**Source:** BIBRA, 2002
**Test substance:** Reported as undecanol Cas# 112-42-5.
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
27-NOV-2004 (10)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male
**No. of Animals:** 6
**Vehicle:** other: air
**Doses:** 0.4 mg/l
**Exposure time:** 6 hour(s)
**Value:** > .4 mg/l

**Method:** other: screening
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None

CLINICAL SIGNS: None

NECROPSY FINDINGS: Unremarkable

**Source:** Younger, 1977
**Conclusion:** Rat 6 hour LC50 >0.4 mg/l (screening test nominal concentration)
**Test condition:** TEST ORGANISMS: rats
- Source: no data
- Number of animals: 6
- Controls: no

ADMINISTRATION: inhalation
- Type of exposure: whole body, 35 litre chamber
- Concentrations: 0.4 mg/l
- Particle size: no data
- Type or preparation of particles: vapour

EXAMINATIONS: Clinical signs, gross necropsy

**Reliability:** (2) valid with restrictions
Screening test with basic information and result reporting, appears valid.

27-NOV-2004 (43)

### 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Value:** > 5000 mg/kg bw

**Method:** other: no information provided
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Limited documentation on study design. Secondary reference reporting unpublished data.
**Flag:** Critical study for SIDS endpoint
31-AUG-2004 (26)

**Type:** LD50
**Species:** rabbit
**Value:** = 4.76 ml/kg bw

**Test substance:** other TS: Reported as undecanol no further details of composition/purity.

**Reliability:** (4) not assignable
Secondary reference
13-OCT-2004 (28)

**Type:** LD50
**Species:** guinea pig
**Vehicle:** other: undiluted
**Value:** > 20 ml/kg bw

**Method:** other: Smyth & Carpenter, 1944
**Year:** 1944
**Test substance:** other TS: Reported as undecanol no further details of

composition/purity.

**Remark:** Application was on absorbent cotton wool to guinea pig skin for 4 days. The authors state that they don't place confidence in results with the guinea pig test where dosages are greater than 5 ml/kg, which is the case in this instance.
**Reliability:** (3) invalid
Screening study limited result reporting but probably valid.
26-OCT-2004 (10) (16) (27) (32)

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: undiluted
**Doses:** 2000, 3160, 5010 and 7940 mg/kg
**Value:** > 3160 - 5000 mg/kg bw

**Method:** other: screening
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: 3-4 days after dosing.
- Number of deaths at each dose: 2000 (0/1), 3160 (0/1), 5010 (1/1) and 7940 (1/1) mg/kg

APPLICATION SITE: Nothing reported

CLINICAL SIGNS: Reduced appetitie and activity (2-4 days in survivors) increasing weakness, collapse and death.

NECROPSY FINDINGS: Survivors: unremarkable. Decedendents: haemorrhagic lungs; discolouration of the liver, enlarged gall bladder, darkened kidneys and spleen, gastrointestinal inflammation.
**Source:** Younger, 1977
**Test condition:** TEST ORGANISMS: rabbits
- Source: no data
- Group size: 1 rabbit/dose level alternate male female
- Controls: no

ADMINISTRATION: dermal
- Area covered: no data
- Occlusion: no data
- Doses: 2000 (male), 3160 (female), 5010 (male) and 7940 (female) mg/kg
- Removal of test substance: no data

EXAMINATIONS: Clinical signs, gross necropsy.
**Conclusion:** This screening test indicates a rabbit dermal LD50 in excess of 3160 mg/kg (but <5000 mg/kg).
**Reliability:** (2) valid with restrictions
Screening test with basic information and result reporting, probably valid.
11-MAY-2006 (43)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

### 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** other: New Zealand White albino rabbit
**Exposure:** no data
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted (also as 25 and 50% solution in PEG 400)
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1981
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Some of this data is reported in an earlier publication by these authors. Jacobs et al, 1987 (Reg. Tox. Pharm. 7:370-378)
**Result:** AVERAGE SCORE (individual animal scores were not reported)
Undiluted
- Erythema: Group mean 24+48+72 hour score 2.3
- Edema: Group mean 24+48+72 hour score 0.8

50% undecanol in PEG400
- Erythema: Group mean 24+48+72 hour score 2.23
- Edema: Group mean 24+48+72 hour score 0.6

25% undecanol in PEG400
- Erythema: Group mean 24+48+72 hour score 1.53
- Edema: Group mean 24+48+72 hour score 0

REVERSIBILITY: Irritation scores were only reported up to 72 hours after exposure and over this time course the irritant effects were not reversible. Group mean erythema scores increased over this observation period for all test concentrations. For undiluted material erythema scores were as follows 24 hour 1.5; 48 hours 2.4; 72 hour 3, oedema remained constant at 0.8. Erythema scores with the 50% solution increased from 2.2 to 2.8 while the oedema score reduced from 0.8 to 0.2. The 25% solution showed an increase in erythema score from 1.2 to 2.0 there was no oedema.

OTHER EFFECTS: Not reported.
**Source:** Jacobs and Martens 1992.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit

- Strain: New Zealand White
- Number of animals: 6

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted or in polyethylene glycol 400 (PEG400)
- Area of exposure: 6x6 cm
- Occlusion: Under exposure chamber of 6X6 cm
- Vehicle: Undiluted or 25 or 50% in PEG400.
- Exposure period: 4 hours
- Postexposure period: 72 hours
- Removal of test substance: Not reported
- Controls: The skin irritancy of PEG400 was not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours.

**Conclusion:** Following a 4 hour occlusive exposure to rabbit skin undiluted undecanol was found to be irritant according to both EU and GHS (category 2) criteria. 25 and 50% dilutions in PEG400 were also tested, the 50% dilution was irritant under EU criteria while both the 25% and 50% dilutions would be considered mild irritants (category 3) under GHS.

**Reliability:** (2) valid with restrictions
Guideline study with acceptable restriction, reporting of results limited.

**Flag:** Critical study for SIDS endpoint

27-OCT-2004 (21)

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"
**Year:** 1985
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 3 animals scored 2 the remaining 3 scored 1.7. Group mean 24+48+72 hour score 1.83.
- Oedema: Individual 24+48+72 hour scores 3 animals scored 1.3 the remaining 3 scored 1.7. Group mean 24+48+72 hour score 1.5.

REVERSIBILITY: By day 7 all scores for oedema were 0. There was evidence that erythema was also regressing the group mean 7 day score being 1.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS 1985b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White

- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Lial 111 (50% linear)
**Conclusion:** Following a 4 hour occluded exposure to rabbit skin, LIAL 111 (C11) was not a skin irritant according to EU criteria (group mean 24+48+48 hour scores <2). With erythema scores all >=1.5 LIAL 111 is classifiable as a mild (slight) skin irritant according to the GHS.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
11-OCT-2004 (12)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**Result:** moderately irritating

**Method:** Draize Test
**Year:** 1973
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This reference gives a summary of unpublished data submitted in 1973 by Moreno. Limited information on the method indicates that undiluted material was applied to rabbit skin (intact and abraded) using a 24 hour occlusive exposure.
**Result:** 1-undecanol was described as moderately irritating to rabbit skin following a 24 hour occluded exposure.
**Source:** Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
13-OCT-2004 (26) (27)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** no data
**Exposure Time:** 24 hour(s)

**No. of Animals:** 6
**PDII:** 5
**Result:** highly irritating

**Method:** other: FHSA
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hours
- Erythema:
individual intact 3, 3.7, 2, 4, 3, 3 group intact 3.1
individual abraded 3, 3, 2, 4, 3, 3 group abraded 3.0
- Oedema:
individual intact and abraded 2, 2, 2, 2,3, 1,7, 2 group
individual abraded as above

REVERSIBILITY: Both erythema and oedema persisted in 4/6 rabbits to 7 days.

OTHER EFFECTS: A defatting effect was reported. The skin sloughed off within 10 to 14 days. There was no in depth injury

**Source:** Younger, 1977
**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: no data
- Source: no data
- Age: no data
- Number of animals: 6
- Controls: no

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Area of exposure: no data
- Occlusion: not reported, 24 hour exposure to intact and abraded skin.
- Total volume applied: 0.5 ml
- Postexposure period: 14 days
- Removal of test substance: no data

EXAMINATIONS
- Scoring system: FHSA
- Examination time points: 4, 24, 48 and 72 hours and 7 days for scoring, observed until 10 days.

**Conclusion:** With individual mean 24+48+72 hour scores in excess of 2.3 in 5/6 test rabbits and a group mean 24+48+72 hour erythema and oedema scores >2 undecanol is classifiable as a Category 2 skin irritation under GHS criteria and as irritant under EU critieria.
**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
26-OCT-2004 (43)

**Species:** human
**Concentration:** 4 %
**Exposure:** Occlusive
**Exposure Time:** 48 hour(s)

**Vehicle:** petrolatum
**Result:** not irritating

**Method:** other: human closed patch test
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of unpublished data from Kligman, 1973.
**Reliability:** (4) not assignable
Secondary reference
13-OCT-2004 (26)

**Species:** other: rabbit and man
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**Vehicle:** other: polyethylene glycol 400

**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** A 25% concentration of 1-undecanol in PEG 400 was not classifiable as a skin irritant in rabbits while a 50% dilution had no adverse effect on human skin. Individual scores were not reported.
**Test condition:** This study was undertaken to determine a limit concentration (in a non-irritant diluent) at which the test materials would not produce classifiable skin irritation (EU classification). The cut off parameter taken was the highest test concentration at which the 24+48+72 hour group mean erythema score was <2.

A series of alcohols were tested including undecanol.

The test method was similar to OECD 404, using a 4 hour covered application (Finn chamber) to intact and abraded rabbit skin. Graded dilutions (5-100%) in the solvent (PEG 400 for 1-undecanol) were tested and the concentration which did not produce skin irritation at classifiable levels was reported as the limit concentration. Groups of 5-6 rabbits were used for this study.

In some instances (including 1-undecanol) the limit concentration was retested on the upper arm of 2-3 human volunteers using the same protocol.
**Conclusion:** A 25% dilution of 1-undecanol in PEG 400 was not classifiable as irritant to rabbit skin according to EU criteria. A 50% dilution had no adverse effect on human skin therefore the limit concentration is considered to be 50%.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
05-APR-2005 (20)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted

**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Result:** slightly irritating

**Method:** other: US FHSA
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The individual scores were not reported only the calculated Draize scores.

AVERAGE SCORE (24+48+72 hour) 10.3/110 combined cornea, iris and conjunctivae.

DESCRIPTION OF LESIONS: There was immediate slight discomfort with slight redness and copious discharge at 10 minutes which developed to slight to moderate redness with copious discharge at 1 hour. At 24 hours there was barely perceptible corneal dullness, the reaction of the iris to light was sluggish in 2 rabbits (maximum score 1), conjunctival involvement (slight to moderate redness with whitish discharge) was observed in all eyes at this time period.

REVERSIBILITY: After 24 hours there was a gradual improvement through to 120 hours when the iris and cornea appeared normal. All eyes appeared completely normal by 7 days.

**Source:** Younger, 1977
**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: no data
- Number of animals: 6
- Controls: no

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: Draize
- Observation period: Scored at 1, 24, 48, 72, 120 and 168 hours (7 days).

**Conclusion:** Undecyl alcohol is described as slightly irritating to the eye in this test. Under GHS criteria the results suggest classification as mild. Under EU criteria undecyl would not be considered irritant.
**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (43)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** other: various
**Comment:** not rinsed
**No. of Animals:** 5

**Method:** other: Carpenter & Smyth, 1946
**Year:** 1946
**GLP:** no
**Test substance:** other TS: reported as undecanol no other details

**Result:** Undecanol was classified as group 3 (0.5 ml undiluted yields score of >5 and 0.1 ml yields not greater than 5.
**Test condition:** This eye irritation assay involves treating the eye with different volumes and concentrations of the test substance and evaluating the corneal and iritic effects after 18-24 hours before and after fluorescein staining (score maximum 20). A score of 5 is considered to represent severe injury. A 10 point grading scale incorporating the scores at various dilutions and volumes is used to classify the observed effects.
**Reliability:** (3) invalid
Non standard method as described above, not comparable with modern guidelines, not considered vaild for classification of irritation.

18-JUL-2005 (13)

## 5.3 Sensitization

**Type:** other: human maximisation test
**Species:** human
**No. of Animals:** 25
**Vehicle:** petrolatum
**Result:** not sensitizing

**Method:** other: human maximisation test
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of a human maximisation test. tested in 25 human volunteers at 4% in petrolatum undecanol produced no sensitisation reactions. Unpublished data from Kligman dated 31st October 1973.
**Reliability:** (4) not assignable
Secondary reference

13-OCT-2004 (26)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for undecanol from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A) and 1-hexadecanol. The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific

systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (19) (30) (36)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Bacillus subtilis recombination assay
**Concentration:** maximum 20 ul/disc
**Result:** positive

**Method:** other
**Year:** 1986
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The spore rec-assy with B. subtilis strains 45 (rec-) and H17 (rec+) was used to detect DNA damaging activity by differences in growth inhibition zones ( D in mm = M45-H17). The maximum dose used was 20 ul/disc.

The result was positive, D being 13. This was equivalent to a +++ response using a 3 step classification where 12<= D equates to +++.
**Source:** Yoo, 1986
**Conclusion:** N-undecyl alcohol gave a positive response in t = B. subtilis rec assay.
**Reliability:** (4) not assignable
Original in Japanese, no translation available.
26-OCT-2004 (27) (42)

**Type:** Escherichia coli reverse mutation assay
**System of testing:** E. coli WP2 uvrA (trp-)
**Concentration:** 0.005 - 0.04 mg/plate
**Cytotoxic Concentration:** no datano data
**Metabolic activation:** no data
**Result:** negative

**Method:** other
**Year:** 1986
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No further experimental detail available from the English summary. The result was negative with a reversion ratio of 1.2.
**Source:** Yoo, 1986
**Conclusion:** Undecanol did not increase the reverse mutation rate in the E. coli test strain WP2 uvrA (trp -).
**Reliability:** (4) not assignable
Original in Japanese, no translation available.

26-OCT-2004 (42)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 - C24-34) including data for 1-octanol, 1-decanol, C10-16 (types B&C) dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are either guideline or similar studies or publications with sufficient detail for assessment.

14-SEP-2005 (19) (30) (31) (36)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C11 alcohol (1-undecanol) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** no expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for

assessment.

14-SEP-2005 (19) (30) (31) (36)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that undecyl alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (19) (30) (31) (36)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: aspiration

**Remark:** Following aspiration of 0.2 ml 1-undecanol all ten treated rats died within 1-10 minutes.
**Test substance:** As prescribed 1-undecanol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

13-OCT-2004 (17)

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(4) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

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(7) Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 112-70-9 |
| **CAS No.** | 112-70-9 |
| **EINECS Name** | tridecan-1-ol |
| **EC No.** | 203-998-8 |
| **TSCA Name** | 1-Tridecanol |
| **Molecular Formula** | C13H28O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **50** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

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02-AUG-2005

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23-AUG-2005

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**Remark:** Consortium Member
19-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

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19-DEC-2005

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**Type:** cooperating company
**Name:** Shell Chemical Company
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**Remark:** Consortium Member
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**Name:** Shell Chemicals Limited
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**Type:** cooperating company
**Name:** The Procter & Gamble Company
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**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |

| | |
|---|---|
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set. For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other
cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results.In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

19-SEP-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Tridecanol
**Smiles Code:** OCCCCCCCCCCCCC
**Mol. Formula:** C13 H28 O1
**Mol. Weight:** 200.37

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-tridecanol, CAS 112-70-9 are >80% linear.

The substance comprises >90% C13. Components of even and odd chain length, in the range C12-C14 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Tridecanol (6CI, 8CI, 9CI) (CA INDEX NAME)
n-Tridecan-1-ol
n-Tridecanol
n-Tridecyl alcohol
NSC 5252
Tridecyl alcohol
Tridecan-1-ol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in

dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-tridecanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (9) (21) (31)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Paints, Lacquers and Varnishes
19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common

oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-tridecanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
11-AUG-2003

## 2.1 Melting Point

**Value:** = 32 - 33 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (37)

**Value:** = 30.6 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment.
11-OCT-2005 (20)

## 2.2 Boiling Point

**Value:** = 276 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (20)

**Value:** = 152 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test conducted at a pressure of 14 mmHg
**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
11-OCT-2005 (28)

**Value:** = 155 - 156 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** by comparison with other results, it is possible that this BP was measured at a reduced pressure.
**Reliability:** (4) not assignable
11-OCT-2005 (37)

## 2.3 Density

**Value:** = .82

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable

**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (37)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00057 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (12)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 5.51

**Method:** other (measured): Measured values were taken from earlier studies.
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for octanol-water partition coefficient data.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (15) (36)

**Partition Coeff.:** octanol-water
**log Pow:** = 5.82

**Method:** other (measured): Details of method not stated.
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. The original source is not stated.
04-JAN-2005 (2)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .38 mg/l at 20 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The water solubility is estimated to be 0.5 mg/l at a loading

rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (19)

**Solubility in:** Water
**Value:** = .5 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.5 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
09-AUG-2005 (3)

**Solubility in:** Water
**Value:** = .33 mg/l at 25 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
21-SEP-2005 (33)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 19.60746E-12 cm3/molecule.sec
Half-life: 19.6 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

### 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
10-JAN-2005

### 3.1.3 Stability in Soil

**-**

### 3.2.1 Monitoring Data (Environment)

**Method:** The EU samples were obtained during 2001-2 from municipal waste water treatment plants. Each was obtained over a 24-hour period, and preserved by addition of formalin at the time of sampling.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivatisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Samples from Canada were grab samples obtained during August 2003, and were preserved with formalin.

**Remark:** Results for all carbon numbers are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.
The study is of effluent monitoring of 20 biofilm and activated sludge wastewater treatment plants from Europe (12) and Canada (8) receiving predominantly municipal effluent. Concentrations of alcohols and alcohol ethoxylates were measured.

**Result:** In the results, Provinces are indicated as 2-letter abbreviations. Results are presented as µg/L concentrations as:

| Location: Treatment Type | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Vernon, BC: TF | 0.393 | 0.174 | 0.428 | 0.886 | 0.452 | 0.718 | 3.051 |
| Kelowna, BC: AS | 0.243 | 0.102 | 0.107 | 0.181 | 0.095 | 0.121 | 0.849 |
| Toronto, ON: AS | 0.027 | 0.235 | 0.548 | 0.312 | 0.883 | 0.492 | 2.497 |
| La Prairie, QC: AS | 0.070 | 0.030 | 0.029 | 0.041 | 0.057 | 0.068 | 0.295 |
| Victoriaville, QC: AS | 0.069 | 0.019 | 0.014 | 0.048 | 0.026 | 0.109 | 0.285 |
| Paris, ON, AS | 0.036 | 0.030 | 0.033 | 0.059 | 0.083 | 0.060 | 0.301 |
| Cardston, AB: RBC | 1.251 | 0.961 | 3.354 | 3.257 | 3.180 | 2.174 | 14.2 |
| Waterloo, ON: AS | 0.301 | 0.122 | 0.156 | 0.172 | 0.160 | 0.127 | 1.038 |

TF = trickling filter
AS = activated sludge
RBC = rotating biological contactor

Data from activated sludge plants in Europe:

| Total alcohol µg/L Location | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Northwich, UK | 0.468 | 0.319 | 0.305 | 0.154 | 0.485 | 0.591 | 2.322 |
| Cannock, UK | 0.104 | 0.087 | 0.069 | 0.084 | 0.179 | 0.318 | 0.841 |
| Rushmoor, UK | 0.134 | 0.104 | 0.095 | 0.125 | 0.338 | 0.408 | 1.204 |
| Kralingse Veer, NL | 0.410 | 0.147 | 0.138 | 0.125 | 0.368 | 0.138 | 1.326 |
| De Meern, NL | 0.282 | 0.208 | 0.174 | 0.155 | 0.472 | 0.239 | 1.53 |
| Horstermeer, NL | 0.360 | 0.211 | 0.212 | 0.136 | 0.598 | 1.209 | 2.726 |
| Estepona, ES | 0.214 | 0.073 | 0.182 | 0.148 | 0.999 | 1.144 | 2.76 |
| La Vibora, ES | 1.179 | 0.533 | 1.741 | 1.181 | 4.172 | 2.426 | 11.23 |
| Munich, DE | 0.010 | 0.023 | 0.007 | 0.034 | 0.005 | 0.008 | 0.087 |
| Torino, IT | 0.070 | 0.094 | 0.057 | 0.058 | 0.419 | 0.038 | 0.736 |
| Robecco, IT | 0.092 | 0.130 | 0.072 | 0.206 | 0.187 | 0.266 | 0.953 |
| Ratingen, DE | 0.046 | 0.052 | 0.033 | 0.083 | 0.037 | 0.068 | 0.319 |

(usual country and US state designators)

**Reliability:** (2) valid with restrictions
Non-GLP monitoring studies conducted to a high standard

21-DEC-2005 (11)

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 200.4
Data temperature 25 deg C
Log Kow 5.51
Water Solubility 0.38 mg/l
Vapour pressure 0.057 Pa
Melting point 32 deg C
half life in air 19.6 h
half life in water and soil 720 h
RESULTS:
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 2.02% |
| Soil | 95.5% |
| Water | 0.33% |
| Fish | 5.39E-03% |
| Sediment | 2.12% |

The Level III program has also been used, with the default model, using the same input parameters.
The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 69.1 | 0.018 | 0.000171 |
| % in water | 1.36 | 9.38 | 0.0121 |
| % in sediment | 13.1 | 90.6 | 0.117 |
| % in soil | 16.4 | 0.00428 | 99.9 |

The results reflect that the ultimate fate of 1-tridecanol is dependent on its route of release into the environment.
1-Tridecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.
In water, the adsorption coefficient of 1-tridecanol resultsin significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of

these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 5.51 was used in the TGD calculation methods.

**Result:** TGD Hydrophobics method: Koc = 36600
TGD Non-hydrophobics method: Koc = 7680
TGD Alcohols method: Koc = 450
SRC PCKOCWIN method: Koc = 600

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

28-DEC-2005 (5)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (5)

**Method:** Laboratory continuous activated sludge study.

4 mg/L of TS
20°C
Hydraulic residence time (HRT) 6 h

Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.

**Remark:** This paper describes mainly the properties of alcohol ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.

**Result:** Results are corrected for control values.

| Alcohol | Conc. in effluent ng/L | Conc. in sludge µg/g | %removal |
|---|---|---|---|
| C12 | 18 | 0.6 | 98.6 |
| C13 | 21 | 0.7 | 99.5 |
| C14 | 5.5 | 0 | 99.6 |
| C15 | 2.9 | 1.1 | 99.8 |
| C16 | 1.6 | 0.01 | 99.5 |
| C18 | 58 | 0.7 | 99.1 |
| Total | 130 | 2 | 99.4 |

| | |
|---|---|
| Total elimination of ethoxylates | 97.4 |
| Total in waste sludge solids | 2.0 |
| Total in suspended solids | 0 |

This shows that most of that which does not degrade (itself a small amount) is in the solids.

**Test substance:** 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

| C | Mol ratio |
|---|---|
| 12 | 1 |
| 13 | 2 |
| 14 | 2.3 |
| 15 | 1.8 |
| 16 | 1.1 |
| 18 | 2.9 |

**Reliability:** (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

21-DEC-2005 (29)

**Method:** Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation Liquid-chromatography-mass spectrometric (LCMS) technique.

**Result:** Influent (In), effluent (Eff) values in ug/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

| | | C12-15 OH | | | C16-18 OH | | |
|---|---|---|---|---|---|---|---|
| | WWTP type | In | eff | % | in | eff | % |
| TX | Lagoon | 297 | 2 | 99.3 | 92.7 | 2.4 | 97.4 |
| NJ | Oxidation Ditch | 249 | 0.7 | 99.7 | 181 | 0.8 | 99.6 |
| OH | Rotating biological contactor | 157 | 0.1 | 0.06 | 77 | 0.07 | 99.9 |
| IA | Trickling filter | 499 | 2.0 | 99.6 | 354 | 2.3 | 99.4 |
| MO | Trickling filter | 532 | 4.9 | 99.1 | 315 | 9 | 97.3 |
| KS | Lagoon | 67.5 | 1.1 | 98.4 | 35.4 | 2.2 | 93.8 |
| CA | Activated sludge | 20.05 | 0.2 | 99.9 | 169 | 0.4 | 99.8 |
| OR | Activated sludge | 92.9 | 0.2 | 99.8 | 133 | 0.6 | 99.5 |
| AZ | Oxidation ditch | 702 | 0.3 | 100 | 394 | 0.5 | 99.9 |

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP studies conducted to a high standard.

21-DEC-2005 (25)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 9630

**Method:** other: calculated (Veith et al, 1979)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 5.51 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

21-DEC-2005 (5)

## 3.8 Additional Remarks

**-**

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** > .33
**Limit Test:** no

**Method:** other: USEPA 1975.
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Both Veith et al citations have the same authors and report the same data. In the papers, the solubility of tridecanol is cited as 0.33 mg/l. An LC50 was not achieved at the solubility limit.
**Result:** No fish mortality was observed in saturated solution. The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.
**Test condition:** TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.

MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-JAN-2005 (34) (35)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The test substance is predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = .51

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.

The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.
**Source:** Unilever. 1995.
**Reliability:** (4) not assignable
This is key study as it is the only one for C13 effects on invertebrates. However no details are available.
**Flag:** Critical study for SIDS endpoint
19-OCT-2005 (30)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The test substance is predicted to be non-toxic at the limit of solubility
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (7)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 3.13

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
The MIC concentration appears to be above the SPARC estimated water solubility of Tridecanol.
**Source:** Hattori 1987.
**Reliability:** (3) invalid
11-OCT-2005 (16)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)
**Unit:** µg/l **Analytical monitoring:**
**NOEC:** = 6 - 46 calculated

**Method:** other: calculated (QSAR)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater

than C15, no chronic effects would be expected.

Structure-activity relationships have been developed based on these results. It is possible to apply these structure-activity relationships to estimate chronic toxicity endpoints where there are no reliable measured data.

Two QSAR relationships have been developed. It can be concluded that the NOEC for reproduction would be within the range of the two estimates.

**Result:** It can be estimated that chronic NOEC(reproduction) for Daphnia magna would lie in the range of 0.006 - 0.046 mg/l.

**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (8)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized

by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (13)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: Carworth-Wistar
**Sex:** male
**Value:** = 17.2 ml/kg bw

**Method:** other: Smyth et al, 1982
**Year:** 1962
**Test substance:** other TS: mixed primary isomers of tridecanol

**Remark:** Variously reported in secondary references, RTECS LD50 17.2 g/kg, HSDB and Patty LD50 17.2 ml/kg (correctly), BIBRA LD50 ca 15 g/kg (conversion).
**Result:** The rat oral LD50 for tridecanol mixed primary isomers is 17.2 ml/kg (confidence limits 12.3-23.9 ml/kg). equivalent to 13,760 mg/kg using the density of 0.82 g/cm3, reported in chapter 2.3. No further details are given.
**Test condition:** TEST ORGANISMS: rats
- Source: no data
- Age: 4-5 weeks
- Weight at study initiation: 90-120 g
- Group size: 5 males/group
- Controls: no

ADMINISTRATION: gastric intubation of either the undiluted material or a solution in water or cornoil or as an agar suspension.
- Doses: logarithmic series differing by a factor of 2.
- Doses per time period: single
- Volume administered or concentration: no data
- Post dose observation period: 14 days

EXAMINATIONS: clinical observations.
**Reliability:** (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.
11-MAY-2006 (10) (17) (22) (24) (27)

**Remark:** Unpublished data cited by BIBRA 1988. No overt toxic effects were observed when 2g/kg was administered to a group of 5 rats. LD50 >2 g/kg. No further data available.
**Test substance:** Tridecanol 50% branched chain primary isomers
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
27-NOV-2004 (10)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Groups of 6 rats were exposed to the concentrated vapours of the test material for periods up to 8 hours. All rats survived this exposure.

This study is also reported in secondary references, RTECS, 2004, HSDB, 2004, Patty, 1982
**Test substance:** mixed primary isomers of tridecanol
**Reliability:** (4) not assignable
Screening test only, gives some indication of toxicity, insufficient documentation.
27-OCT-2004 (17) (22) (24) (27)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male
**Vehicle:** no data
**Value:** = 7.07 ml/kg bw

**Method:** other: Smyth et al, 1962
**Year:** 1962
**GLP:** no
**Test substance:** other TS: mixed isomers of tridecanol

**Result:** The rabbit dermal LD50 for mixed primary isomers of tridecanol was 7.07 ml/kg (confidence limits 2.33-21.4 ml/kg). Equivalent to 5797 mg/kg using the density of 0.82 g/cm3, reported in chapter 2.3. This result is also cited by Patty 1982 and HSDB 2004.
**Test condition:** The test substance was applied to the shorn skin of groups of 4 male rabbits under and occlusive dressing for 24 hours. The rabbits were observed for 14 days.
**Reliability:** (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.
11-MAY-2006 (17) (22) (27)

**Remark:** Rabbit dermal LD50 is reported as 5600 mg/kg. No further details available. (The value reported could be a conversion to mg/kg of the LD50 of 7.07 ml/kg reported by Smyth et al, 1962 as the density is in the region of 0.8.)
**Test substance:** Reported as Cas# 112-70-9 but no information on isomeric content.
**Reliability:** (4) not assignable
Secondary reference, value reported in NPIRI Handbook 1974.
27-NOV-2004 (24)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Open
**Exposure Time:** 24 hour(s)
**No. of Animals:** 5
**Result:** slightly irritating

**Method:** other: Smyth et al, 1962
**Year:** 1962
**GLP:** no
**Test substance:** other TS: mixed primary isomers of tridecanol

**Result:** Skin irritation is grade 4 which is described as producing slight erythema.
**Test condition:** This is a non-standard test. The test material is applied for a 24 hour uncovered exposure in a volume of 0.01 ml of either the undiluted material or dilutions in water or solvent. For this test the material was applied undiluted. Skin irritation is graded on a 10 point scale (this is described fully in Smyth et al, 1949)
**Reliability:** (3) invalid
Non standard method not comparable to modern guidelines.
27-OCT-2004 (27)

**Remark:** In an open irritation test on rabbit skin 410 mg tridecanol was reported to produce a mild irritant effect. No further details available.
**Test substance:** Reported as tridecanol in RTECS under Cas# 112-70-9 no details of isomeric content.
**Reliability:** (4) not assignable
Secondary reference to Union Carbide SDS, 1964 unobtainable.
28-OCT-2004 (24)

### 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** other: various
**Comment:** not rinsed

**Method:** other: Carpenter & Smyth, 1946
**Year:** 1946
**GLP:** no
**Test substance:** other TS: mixed primary isomers of tridecanol

**Result:** In this test tridecanol was classified as grade 2 (0.5 ml undiluted gives injury of >1-5 points. <1 indicates at most a very small area of necrosis. Irritation might be considered as moderate to severe.

This result is also reported in Patty, 1982, BIBRA, 1988 and HSDB, 2004.

**Test condition:** This eye irritation test is based on a protocol developed in 1946 (Carpenter & Smyth, 1946). This eye irritation assay involves treating the eye with different volumes and concentrations of the test substance and evaluating the corneal and iritic effects after 18-24 hours before and after fluorescein staining (score maximum 20). A score of 5 is considered to represent severe injury. A 10 point grading scale incorporating the scores at various dilutions and volumes is used to classify the observed effects.
**Reliability:** (3) invalid
Non standard method as described above, not comparable with modern guidelines, not considered valid for classification of irritation.
27-OCT-2004 (27)

**Remark:** Unpublished data cited by BIBRA 1988. One drop of the test substance produced no effects in rabbits. No further details available.
**Test substance:** Tridecanol 50% branched chain primary isomers
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
14-SEP-2005 (10)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are indicating lack of sensitisation potential are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for, C6 (hexanol), C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A) and C14 (tetradecanol) alcohols which support the conclusion that 1-Tridecanol is not expected to be a skin sensitiser.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
05-DEC-2005 (26) (32)

## 5.4 Repeated Dose Toxicity

**Species:** rat **Sex:** male
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 14 days
**Frequency of treatment:** daily
**Post exposure period:** no
**Doses:** 1 mmol/kg/day (184 mg/kg/day)
**Control Group:** yes, concurrent vehicle

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** other TS: Tridecanol branched

**Result:** In vivo studies: There were no effects on relative testes weight, relative liver weight showed a slight* significant increase with 3,5,7-trimethyl hexanol. The postive control DEHP showed a clearly significant increase** in relative liver weight. There were no significant changes in testes weight relative to controls. Histopathological examination of the liver revealed no treatment related changes. Only the positive control DEHP showed any peroxisome proliferation or effects on cholesterol or triglycerides catalase was unaffected by treatment.
In vitro levels of palmitoyl CoA oxidase were increased only in the positive control group (MEHP).

**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce similar effects to those observed with diethyl hexyl phthalate (DEHP) and its metabolite 2-ethyl hexanol in terms of hepatomegaly, peroxisome proliferation, hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any indication of testicular atrophy (a known effect of DEHP).

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol 300 as a vehicle and the test compounds at a common dose level (on a molar basis) of 1 mmol/kg/day for 14 days. At the end of this period liver and testes weights were recorded. The liver was removed and samples taken for light and electron microscopy. The remaining liver was homogenised and prepared for assay of total catalase and CN-insensitive palmitoyl CoA oxidation. In vitro hepatocyte cultures were also prepared and the same compounds assessed for effects on CN-insensitive palmitoyl CoA oxidase activity after 72 hours incubation.
Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day

**Test substance:** Materials tested were as follows:

Branched alcohols
2-ethyl hexanol C8
Iso-octanol C8
3,5,7-trimethylhexanol C9
Iso-nonanol C9
Iso-decanol C10
Tridecanol C13

Mixed branched & straight chain
Alphanol C7-9

Synprol C13-15 CAS RN 67762-41-8
Straight chain
Alfol C6-10 (Alfol 610) C6-10 (even) CAS RN 64365-05-5
Linevol C7-9 (Linevol 79) (even & odd) CAS RN 68603-15-6 (85% linear).

**Conclusion:** None of the alkanols investigated at dose levels of 1 mMol/kg showed any evidence of peroxisome proliferation, hepatomegaly, hepatomegaly, or hypolipidaemia. Testes weights were also unaffected by treatment.

Study cited by BIBRA, 1988.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

28-OCT-2004 (10) (23)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for 1-tridecanol are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (26) (32)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
14-SEP-2005 (1) (18) (26) (32)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

-

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that 1-tridecanol is not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (1) (26) (32)

## 5.8.3 Toxicity to Reproduction, Other Studies

**Type:** other: comparative study including measurement of testes weight
**In Vitro/in vivo:** In vivo
**Species:** rat
**Strain:** Wistar **Sex:** male
**Route of administration:** gavage
**Exposure period:** 14 days
**Frequency of treatment:** daily
**Duration of test:** 14 days
**Doses:** 1 mmol/kg/day (184 mg/kg/day for tridecanol)
**Control Group:** yes, concurrent vehicle

**Method:** other: see text
**Year:** 1984
**GLP:** no data

**Test substance:** other TS: Tridecanol branched

**Result:** Following repeated oral administration of equimolar dose levels of various alkanols to male rats for a period of 14 days there were no statistically significant differences in body weight gain, or relative liver or testes weights.

**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce similar effects to those observed with diethyl hexyl phthalate (DEHP) and its metabolite 2-ethyl hexanol in terms of hepatomegaly, peroxisome proliferation, hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any indication of testicular atrophy (a known effect of DEHP).

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol as a vehicle at a common dose level (on a molar basis) of 1 mmol/kg/day for 14 days. At the end of this period testes weights were recorded together with various indices of liver toxicity (see chapter 5.4 Repeated dose toxicity for further details).

Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day

**Conclusion:** The results of this study provide supportive evidence for a lack of effect of a range of alcohols on the testes following repeated oral administration as evidenced by lack of effect on relative testes weights.

**Reliability:** (2) valid with restrictions
Research study well documented, meets generally accepted scientific principles, acceptable for assessment.

06-AUG-2005 (10) (23)

## 5.9 Specific Investigations

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## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: aspiration

**Remark:** Following aspiration of 0.2 ml n-tridecanol 9/10 treated rats died within 2 hours following severe dyspnea.

**Test substance:** n-tridecanol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

28-OCT-2004 (14)

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(4) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(5) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(6) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(7) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(8) Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

(9) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 112-72-1
**CAS No.** 112-72-1
**EINECS Name** tetradecanol
**EC No.** 204-000-3
**TSCA Name** 1-Tetradecanol
**Molecular Formula** C14H30O

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
**Revision date:**
**Date of last Update:** **11-MAY-2006**

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**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK, The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

03-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** industry consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |

| | |
|---|---|
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Tetradecanol
**Smiles Code:** OCCCCCCCCCCCCCC
**Mol. Formula:** C14 H30 O1
**Mol. Weight:** 214.39
21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-tetradecanol, CAS 112-72-1 are 100% linear.

The substance comprises >95% C14. Components of even chain length, in the range C12-C16 are present.
05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Tetradecanol (8CI, 9CI) (CA INDEX NAME)
Tetradecanol (7CI)
Alcohol C-14
Tetradecan-1-ol
Some commercial products with the name CO
Some commercial products with the name Lorol
Lanette Wax KS
Loxanol V
Myristic alcohol
Myristyl alcohol
n-Tetradecan-1-ol
n-Tetradecanol
n-Tetradecyl alcohol
Nacol 14-95
NSC 8549
Tetradecyl alcohol
1-Hydroxytetradecane
1-Tetradecyl alcohol
Adol 18
Alfol 14

Conol 1495
Kalcohl 40
Kalcohl 4098
Lanette 14

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-tetradecanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (7) (49) (76)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.
The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 35 Lubricants and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available
19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (80)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-tetradecanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available
For full details of search strategy, refer to SIAR Section 7.
03-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
03-AUG-2005

## 2.1 Melting Point

**Value:** = 39.5 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. Original reference not stated.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (81)

**Value:** = 39.5 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
Assessment performed according to accepted models and principles.
21-OCT-2005 (71)

**Value:** = 38 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment.
21-OCT-2005 (47)

**Value:** = 35 - 38 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
21-OCT-2005 (59)

**Value:** = 37.4 - 37.7 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint
21-OCT-2005 (59)

**Value:** = 37.8 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
21-OCT-2005 (16)

**Value:** = 38 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
21-OCT-2005 (38)

## 2.2 Boiling Point

**Value:** = 289 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (46)

**Value:** = 263.2 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (81)

**Value:** = 264 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (52)

**Value:** = 280 - 300 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (59)

**Value:** = 285 - 300 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (59)

**Value:** = 296.2 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (9)

## 2.3 Density

**Type:** density
**Value:** = .8236 g/cm³ at 38 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (38)

**Type:** density
**Value:** = .8355 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning

this endpoint.
11-OCT-2005 (61)

**Type:** density
**Value:** = .81 - .82 g/cm³ at 40 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
11-OCT-2005 (59)

**Value:** = .823 g/cm³

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
21-OCT-2005 (77)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00014 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (14)

**Value:** = .0133 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (61)

**Value:** = .00015 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
09-AUG-2005 (3)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 6.03

**Method:** other (measured): Reverse-phase HPLC with mass spectrometry
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
**Test condition:** Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm. Mobile Phase: Solution A: methanol:ethanol:water 70:15:15. Solution
B: methanol:ethanol:water 95:5:0 100% A for 1 min Gradient to 100% B at 6.67% per min 100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).
**Reliability:** (2) valid with restrictions
Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (10)

**Partition Coeff.:** octanol-water
**log Pow:** = 6.36

**Method:** other (measured): details of method not stated
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original source not stated.
04-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .191 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered authoritative for water

solubility values.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (71) (84)

**Solubility in:** Water
**Value:** = .35 mg/l at 25 degree C

**Method:** other: measured (keine weiteren Angaben)
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. However, the source of the value is a recognised source of physico-chemical data. This reference is considered authoritative for water solubility values.
11-OCT-2005 (83)

**Solubility in:** Water
**Value:** = .31 mg/l

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
11-OCT-2005 (46)

**Solubility in:** Water
**Value:** .2 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.202 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
11-OCT-2005 (3)

**Value:** = .31 mg/l at 25 degree C

**Method:** other: measured (ueber Oberflaechenspannung)

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
11-OCT-2005 (56)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 140 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Whilst not stated, it is considered likely that this is a result from a closed-cup test, by comparison with other measured values.
**Reliability:** (4) not assignable
This value was obtained from secondary literature.
04-JAN-2005 (40)

**Value:** ca. 155 degree C
**Type:** open cup

**Method:** other: DIN 51758/ISO 2719
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
04-JAN-2005 (59)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
04-JAN-2005

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
04-JAN-2005

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
04-JAN-2005

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Viskositaet (40 Grad C): 12.9 mPa * s
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM
04-JAN-2005 (69)

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 21.02050E-12 cm3/molecule.sec
Half-life: 18.3 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

### 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
10-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

**Method:** The EU samples were obtained during 2001-2 from municipal waste water treatment plants. Each was obtained over a 24-hour period, and preserved by addition of formalin at the time of sampling.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivatisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Samples from Canada were grab samples obtained during August 2003, and were preserved with formalin.
**Remark:** The study is of effluent monitoring of 20 biofilm and activated sludge wastewater treatment plants from Europe (12) and Canada (8) receiving predominantly municipal effluent. Concentrations of alcohols and alcohol ethoxylates were measured.

**Result:** In the results, Provinces are indicated as 2-letter abbreviations. Results are presented as µg/L concentrations as:

| Location: Treatment Type | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Vernon, BC: TF | 0.393 | 0.174 | 0.428 | 0.886 | 0.452 | 0.718 | 3.051 |
| Kelowna, BC: AS | 0.243 | 0.102 | 0.107 | 0.181 | 0.095 | 0.121 | 0.849 |
| Toronto, ON: AS | 0.027 | 0.235 | 0.548 | 0.312 | 0.883 | 0.492 | 2.497 |
| La Prairie, QC: AS | 0.070 | 0.030 | 0.029 | 0.041 | 0.057 | 0.068 | 0.295 |
| Victoriaville, QC: AS | 0.069 | 0.019 | 0.014 | 0.048 | 0.026 | 0.109 | 0.285 |
| Paris, ON, AS | 0.036 | 0.030 | 0.033 | 0.059 | 0.083 | 0.060 | 0.301 |
| Cardston, AB: RBC | 1.251 | 0.961 | 3.354 | 3.257 | 3.180 | 2.174 | 14.2 |
| Waterloo, ON: AS | 0.301 | 0.122 | 0.156 | 0.172 | 0.160 | 0.127 | 1.038 |

TF = trickling filter
AS = activated sludge
RBC = rotating biological contactor

Data from activated sludge plants in Europe:

| Total alcohol µg/L Location | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Northwich, UK | 0.468 | 0.319 | 0.305 | 0.154 | 0.485 | 0.591 | 2.322 |
| Cannock, UK | 0.104 | 0.087 | 0.069 | 0.084 | 0.179 | 0.318 | 0.841 |
| Rushmoor, UK | 0.134 | 0.104 | 0.095 | 0.125 | 0.338 | 0.408 | 1.204 |
| Kralingse Veer, NL | 0.410 | 0.147 | 0.138 | 0.125 | 0.368 | 0.138 | 1.326 |
| De Meern, NL | 0.282 | 0.208 | 0.174 | 0.155 | 0.472 | 0.239 | 1.53 |
| Horstermeer, NL | 0.360 | 0.211 | 0.212 | 0.136 | 0.598 | 1.209 | 2.726 |
| Estepona, ES | 0.214 | 0.073 | 0.182 | 0.148 | 0.999 | 1.144 | 2.76 |
| La Vibora, ES | 1.179 | 0.533 | 1.741 | 1.181 | 4.172 | 2.426 | 11.23 |
| Munich, DE | 0.010 | 0.023 | 0.007 | 0.034 | 0.005 | 0.008 | 0.087 |
| Torino, IT | 0.070 | 0.094 | 0.057 | 0.058 | 0.419 | 0.038 | 0.736 |
| Robecco, IT | 0.092 | 0.130 | 0.072 | 0.206 | 0.187 | 0.266 | 0.953 |
| Ratingen, DE | 0.046 | 0.052 | 0.033 | 0.083 | 0.037 | 0.068 | 0.319 |

(usual country and US state designators)
Results for all carbon numbers are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP monitoring studies conducted to a high standard.

21-DEC-2005 (11)

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models

**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 214.4
Data temperature 25 deg C
Log Kow 6.03
Water Solubility 0.191 mg/l
Vapour pressure 0.014 Pa
Melting point 40 deg C
half life in air 18.3 h
half life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 0.33% |
| Soil | 97.3% |
| Water | 0.10% |
| Fish | 5.50E-03% |
| Sediment | 2.16% |

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 38.4 | 0.00395 | 0.000033 |
| % in water | 1.57 | 4.61 | 0.0106 |
| % in sediment | 32.5 | 95.4 | 0.219 |
| % in soil | 27.6 | 0.00284 | 99.8 |

The results reflect that the ultimate fate of 1-tetradecanol is dependent on its route of release into the environment. 1-Tetradecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-tetradecanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (6)

## 3.3.2 Distribution

**Method:** Measurement of the sorption of five alcohols onto a mixture of activated sludge and river water suspended solids.
River water was collected from River Gowy, Ellesmere Port, on two successive days and mixed then sterilised. It contained 12 mg/L suspended solids.

Activated sludge was obtained from a municipal waste water treatment plant. The mixed liquor suspended solids content was determined to be 2940 mg/L. Total organic carbon was 880 mg/L. The mixture was sterilised, allowed to settle, and a simulated effluent was prepared to give 30 mg/L suspended solids. The fraction of organic carbon was 0.167. The vessel was spiked with TS to give ca. 100 µg/L. The test system was stirred for

24 h, which was sufficient to give equilibrium.

The mixed settled activated sludge with river water with up to 72 h equilibration.

**Remark:** The results for five substances are considered alongside each other since the results of the whole study are useful for comparison purposes.
The data for the alcohol ethoxylates obtained in the study do not need to be included in this summary.

**Result:** Alcohol sorption coefficients showed some time dependence, reaching a plateau by 72 h. C15 was found to be an unexplained outlier. The 72 h results were:

| C | 12 | 14 | 15 | 16 | 18 |
|---|---|---|---|---|---|
| Kd | 3000± 80 | 8490± 920 | 3080± 270 | 23800 ±3200 | 78700 ±5400 |
| Koc | 17980 | 50830 | - | 143000 | 471000 |
| log Koc | 4.25 | 4.71 | - | 5.15 | 5.67 |

These data (neglecting the C15) can be interpreted as a QSAR in the usual way as:

Log Koc = 0.11 + 0.77 log Kow

R2 = 0.994

The result is in line with typical QSARs of this type.

**Test substance:** Linear alcohols labelled with 14-C, radiochemical purity 99%

**Reliability:** (2) valid with restrictions
Although not a SIDS end point, this study is considered to be the best study of Koc for these carbon numbers.

21-DEC-2005 (55)

**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 6.03 was used in the TGD calculation methods.

**Result:**
TGD hydrophobics method: Koc = 96500
TGD Non-hydrophobics method: Koc = 14300
TGD Alcohols method: Koc = 710
SRC PCKOCWIN method: Koc = 1110

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4

**Reliability:** (2) valid with restrictions

The value was predicted using accepted calculation methods.
28-DEC-2005 (5)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: activated sludge, predominantly domestic
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 92 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:** 7 day(s) = 67 %
14 day(s) = 84 %
21 day(s) = 88 %
28 day(s) = 92 %
**Control Subst.:** other: Sodium acetate

**Method:** other: ISO 10708 (BODIS)
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test method used is based on OECD test method 301D and the RDA-Blok-Test. Mineral medium was inoculated with activated sludge and stabilized for one week at 20-25 C with continuous stirring. After stabilisation, 200 ml of test medium was filled into 300 ml bottles, aerated until O2 saturation was reached and spiked with test substance by directly weighing into the test vessels. Vessels were filled 2/3, stoppered and shaken continuously at 20-25 C.

Degradation was followed by weekly measurements of BOD using an O2-electrode. Oxygen consumption resulting from biodegradation of the test substance was corrected by oxygen uptake of blank inoculum. Degradation rate was calculated as % BOD/COD.

**Remark:** The validity criteria were fulfilled:
(1) degradation rate
of reference has reached level of 60% within 14 days,
(2) Parallel assays did not differ by more than 20%,
(3) total oxygen consumption in blanks after first week was lower than 3 mg O2 and lower 1 mg O2 in the following weeks and
(4) residual concentration of O2 in the test bottles did not fall below 0.5 mg/l.

**Result:** Kinetic of control substance:
7 days = 75%
14 days = 85%
21 days = 86%
28 days = 86%
The test substance attained >60% degradation within the 10-day window, therefore it can be considered readily biodegradable.

**Test condition:** Concentration of activated sludge: 30 mg dry matter/l
Test volume: 200ml
Temperature: 20-25 C

pH: not reported
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (37)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 57 % after 31 day(s)
**Result:** inherently biodegradable
**Kinetic:**
| | |
|---|---|
| 4 day(s) | = 28 % |
| 10 day(s) | = 47 % |
| 17 day(s) | = 54 % |
| 24 day(s) | = 56 % |
| 31 day(s) | = 57 % |

**Control Subst.:** other: Sodium benzoate

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 310B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** There is no information given on the validity criteria.
**Result:** Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation over the test period, therefore it cannot be considered readily biodegradable.
**Reliability:** (4) not assignable
The information reported is insufficient to assess the validity of this study.
17-OCT-2005 (79)

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 25.4 mg/l related to Test substance
**Degradation:** = 28 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:**
| | |
|---|---|
| 1 day(s) | = 2 % |
| 10 day(s) | = 10 % |
| 20 day(s) | = 23 % |
| 28 day(s) | = 28 % |

**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm

Test (CO2 evolution)"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were met
(1) Parallel assays did not differ by more than 20%,
(2) the reference substance degraded by >60% during the 14 day window,
(3) CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test,
(4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.
**Result:** Kinetic of control substance:
1 days = 20%
10 days = 66%
20 days = 91%
28 days = 105%
The test substance attained <60% degradation over the test period, therefore it cannot be considered readily biodegradable.
**Test condition:** Concentration of activated sludge: 30 mg dry matter/l
Test volume: 3 l
Temperature: 21°C
pH: not reported
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
17-OCT-2005 (48)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 50 mg/l
**Degradation:** = 55 - 66 % after 28 day(s)

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two-phase closed bottle test
**Remark:** Abbauhemmtest: keine Effekte. Animpfung 10 fach höher als Routine BLOK Test (hohe Eigenzehrung IZK) parallel wurde ein Hemmtes durchgeführt CSB= 2.18mg O2/mg AS BSBT=3.14mg O2/mg AS
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 55% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 66% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 63% with parameter % BSB/CSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (29) (35)

**Type:** aerobic
**Inoculum:** activated sludge, domestic

**Concentration:** 50 mg/l
**Degradation:** = 40 - 58 % after 28 day(s)

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Remark:** Abbauhemmtest: keine Effekte.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 58% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 40% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 68% with parameter % BSB/CSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

28-SEP-2005 (30) (36)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 50 mg/l
**Degradation:** = 80 - 82 % after 30 day(s)
**Result:** other: : well biodegradable

**Method:** other: RDA-Test according to Blok (AWU)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft 74-80% BSB30/BSBT ungenügend Restsauerstoff CSB= 2.18 mg O2/mg AS BSBT=3.14mg O2/mg AS
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 82% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 80% with parameter % BSB/ThSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

11-OCT-2005 (27) (31) (33)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 50 mg/l
**Degradation:** = 91 - 91 % after 30 day(s)
**Result:** other: well biodegradable

**Method:** other: RDA-Test according to Blok (AWU)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft 83% BSB30/BSBT ungenügend Restsuerstoff CSB= 2.18mg O2/mg AS BSBT=3.14mg O2/mg AS

**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 91% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 91% with parameter % BSB/ThSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-OCT-2005 (28) (31) (34)

**Method:** Laboratory continuous activated sludge study.

4 mg/L of TS
20°C
Hydraulic residence time (HRT) 6 h
Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.
**Remark:** This paper describes mainly the properties of alcohol ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.
**Result:** Results are corrected for control values.

| Alcohol | Conc. in effluent ng/L | Conc. in sludge µg/g | %removal |
|---|---|---|---|
| C12 | 18 | 0.6 | 98.6 |
| C13 | 21 | 0.7 | 99.5 |
| C14 | 5.5 | 0 | 99.6 |
| C15 | 2.9 | 1.1 | 99.8 |
| C16 | 1.6 | 0.01 | 99.5 |
| C18 | 58 | 0.7 | 99.1 |
| Total | 130 | 2 | 99.4 |

| | |
|---|---|
| Total elimination of ethoxylates | 97.4 |
| Total in waste sludge solids | 2.0 |
| Total in suspended solids | 0 |

This shows that most of that which does not degrade (itself a

small amount) is in the solids.

**Test substance:** 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

| C | Mol ratio |
|---|---|
| 12 | 1 |
| 13 | 2 |
| 14 | 2.3 |
| 15 | 1.8 |
| 16 | 1.1 |
| 18 | 2.9 |

**Reliability:** (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

21-DEC-2005 (72)

**Method:** The study was a batch-mode activated sludge die-away system. Two treatments consisting of 1 litre each of biologically active sludge were prepared for each test substance. The 14-C alcohols were dissolved in methanol, which was diluted in water and dosed into the sludge in 2-litre flasks.

Disappearance of parent, formation and disappearance of metabolites, uptake into biomass and mineralization to 14-C CO2 were monitored over time.

Activated sludge from a municipal WWTP was obtained, and used at 2500 mg/L.

The TS was dosed at 0.05 µM: this is equivalent to 9.3µg/L (C12), 10.0 µg/L (C14), 10.7 µg/L (C16); added to flasks at 20°C.

**Remark:** The results for three substances are considered alongside each other since the results of the whole study are useful to show the consistency of the results.

**Result:** Recoveries were high.

After 48h incubation:

| C | Parent | metabolites | Water | Solids | CO2 |
|---|---|---|---|---|---|
| C12 | 0.8 | 5.9 | 3.5 | 20.7 | 73.9 |
| C14 | 1.3 | 6.3 | 2.0 | 21.0 | 76.7 |
| C16 | 2.6 | 11.5 | 2.1 | 17.0 | 65.3 |

Concentrations were modelled with the equation
C = Ae^(-k1t) + B(e^-k2t)
(a two compartment first order decay model)

| % | A | k1 h-1 | B | k2 h-1 |
|---|---|---|---|---|
| C12 | 82±2 | 113±8 | 9±1 | 0.36±0.1 |
| C14 | 82±2 | 87±5 | 12±1 | 0.30±0.1 |
| C16 | 41±3 | 103±23 | 48±2 | 0.43±0.04 |

The results show the high biodegradability of C12 to 16 alcohols in activated sludge.

**Test substance:** Radiolabelled (14C) C12, C14 and C16 alcohols.

**Reliability:** (2) valid with restrictions
Non-standard study conducted to a scientifically sound method.
21-DEC-2005 (73)

**Method:** Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation Liquid-chromatography-mass spectrometric (LCMS) technique.

**Result:** Influent (In), effluent (Eff) values in ug/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

| | | C12-15 OH | | | C16-18 OH | | |
|---|---|---|---|---|---|---|---|
| | WWTP type | In | eff | % | in | eff | % |
| TX | Lagoon | 297 | 2 | 99.3 | 92.7 | 2.4 | 97.4 |
| NJ | Oxidation Ditch | 249 | 0.7 | 99.7 | 181 | 0.8 | 99.6 |
| OH | Rotating biological contactor | 157 | 0.1 | 0.06 | 77 | 0.07 | 99.9 |
| IA | Trickling filter | 499 | 2.0 | 99.6 | 354 | 2.3 | 99.4 |
| MO | Trickling filter | 532 | 4.9 | 99.1 | 315 | 9 | 97.3 |
| KS | Lagoon | 67.5 | 1.1 | 98.4 | 35.4 | 2.2 | 93.8 |
| CA | Activated sludge | 20.05 | 0.2 | 99.9 | 169 | 0.4 | 99.8 |
| OR | Activated sludge | 92.9 | 0.2 | 99.8 | 133 | 0.6 | 99.5 |
| AZ | Oxidation ditch | 702 | 0.3 | 100 | 394 | 0.5 | 99.9 |

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP studies conducted to a high standard.
21-DEC-2005 (58)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 33900

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 6.03 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (5)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** semistatic
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** >= 1
**LC50:** > 1
**Limit Test:** yes

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The concentration of 1.0 mg/L was reported to be the highest attainable test concentration due to the limited water solubility, therefore the LC50 was not achieved at the solubility limit, (although 1 mg/l is greater than the measured solubility in pure water).

**Result:**
RESULTS: EXPOSED
NOEC > 1.0 mg/l
LC50 > 1.0 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Test condition:**
TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Parkwood Trout Farm, Harrietsham, Kent UK
Weight: 0.90 g
Feeding: Commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 7 days prior to test
Feeding during test: Discontinued 23 hours prior to test
Control group: Control and solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTIONS: Not determined
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels were aerated during test
Alkalinity: 137 mg/l
Hardness: 259 mg/l CaCO3
Conductance: 627 uS/cm
TEST SYSTEM
Concentrations: 1.0 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 14 C
Dissolved oxygen: = 9.0 - 9.9 mg O2/l
pH mean: 7.6-8.2
TEST PARAMETER: Mortality
SAMPLING: Monitoring of test animals for mortality and sub-lethal effects at 3, 6, 24, 48 and 96 hours

MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (82)

**Type:** semistatic
**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC0:** = 10000
**LC50:** > 10000
**Limit Test:** no

**Method:** Directive 92/69/EEC, C.1
**Year:** 1994
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
LC50 = >10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: none

Nature of adverse effects: mortality or sublethal effects
No mortality or sublethal effects were seen
Substance loading is well above the water solubility limit.
**Test condition:** TEST ORGANISMS
Strain: Brachydanio rerio
Supplier: Westaquarium
Wild caught: no
Age/size/weight/loading: not reported
Feeding: Altromin N 1324
Pretreatment: none
Feeding during test: none
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into test vessels followed by 10 sec treatment with blender to disperse poorly soluble test substance.
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Concentrations: 0, 1000, 3000, 10000 mg/l
Renewal of test solution: daily
Exposure vessel type: 5 L aquarium
Number of replicates: 1
Fish per replicate: 10
Test temperature: 20.5 - 22.5C
Dissolved oxygen: 63-95% saturation
pH mean: 7.9-9.4
Adjustment of pH: not reported
Photoperiod: not reported
DURATION OF THE TEST: 96 h
TEST PARAMETER: mortality
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility are available

11-JAN-2005 (70)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 4

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.

The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.
**Source:** Unilever. 1995.
**Reliability:** (4) not assignable
This is a key study as it is the only one available for effects of C14 on invertebrates. However, no details are available and data obtained from secondary literature.
**Flag:** Critical study for SIDS endpoint
19-OCT-2005 (75)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .18 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

21-DEC-2005 (4)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EL50 :** > 10
**Limit Test:** no

**Method:** other: DIN 38412 part 9.
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of water constituents on green algae (Algae gowth-inhibition-test)(L9); DIN 38412 part 9
This method corresponds to the OECD Guideline 201.

**Remark:** The solubility of C14 alcohol (Tetradecanol) is about 0.15 mg/l, therefore the LC50 was not achieved at the solubility limit. The dose-response was found above the solubility, which suggests the possibility of an artefact causing it.

**Result:** RESULTS: EXPOSED
Nominal/measured concentrations: nominal
Effect data/Element values:
ErL0 = 1 mg/l, ErL10 = 2.9 mg/l, ErL50 = >10 mg/l
EbL0 = 0.1 mg/l, EbL10 = 0.28 mg/l, EbL50 = >10 mg/l
Cell density data: cell densities increased from 2.3-7.3*10exp4 cells/ml after 24 hours to the following densities after 96 hours: 2.4*10exp6 (0.1 mg/l), 2*10exp6 (0.6 mg/l), 1.9*10exp6 (1 mg/l), 2.1*10exp6 (3 mg/l) and 2*10exp6 (10 mg/l).
RESULTS CONTROL: cell density increased from 4.7*10exp4 after 24 hours to 2.1*10exp6 cells/ml after 96 hours.

**Source:** Guhl 1992d.

**Test condition:** TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen

Laboratory culture: not reported
Method of cultivation: not reported
Pretreatment: not reported
Controls: without test substance
Initial cell concentration: 1-10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: a stock solution of 0.1 g/l was stirred for 72 hours, filtered and dilutions prepared from the filtrate
STABILITY OF TEST CHEMICAL SOLUTIONS: not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM:
Test type: static test
Loading rates: 0.1, 0.3, 1, 3 and 10 mg/l
Renewal of test solution: None
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 22.5-23 C
pH mean: not reported
Intensity of irradiation: 2000lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
20-OCT-2005 (21)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans MT 5091
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 1.56

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
The MIC concentration appears to be above the SPARC estimated water solubility of Tetradecanol.
**Source:** Hattori 1987.
**Reliability:** (3) invalid
Best study although not a SIDS endpoint.
Study was considered invalid due to significant methodological deficiencies.
11-OCT-2005 (22)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** 10000
**EC50:** > 10000

**Method:** other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Method conforms with OECD Guide-line 209
**Remark:** Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
**Test substance:** Active Matter = 98 %
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
28-SEP-2005 (26) (32)

**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)

**Method:** other: see Test Condition
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** nicht toxisch bei Saettigungskonzentration (photometrische Messung der Wachstumshemmung)
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** Static test; cell growth determined photometrically at 540 nm
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
06-AUG-2005 (63)

**Species:** other bacteria: Clostridium botulinum
**Unit:** mg/l **Analytical monitoring:**
**MIC :** = .6

**Method:** other: static cell multiplication inhibition test according to Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Testdauer: nicht angegeben
**Source:** Henkel KGaA Duesseldorf
**Test condition:** Ethanol als Loesevermittler (<= 2.5 g/l; MIC = 30 g/l); anaerobe Bedingungen
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (41)

**Species:** other bacteria: Mycoplasma gallisepticum
**Exposure period:** 144 hour(s)
**Unit:** mmol/l **Analytical monitoring:**

**NOEC:** >= .064

**Method:** other: statischer Zellvermehrungshemmtest (photometrische Bestimmung des Zellwachstums (560 nm))
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** keine Hemmung bei einer Konzentration von 0.064 mmol/l = 13.7 mg/l
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 37 Grad C; Ethanol als Loesevermittler (< 1 % v/v; nicht toxisch bei dieser Konzentration)
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (17)

**Species:** other bacteria: Mycoplasma pneumoniae
**Exposure period:** 144 hour(s)
**Unit:** mmol/l **Analytical monitoring:**

**Method:** other: statischer Zellvermehrungshemmtest (photometrische Bestimmung des Zellwachstums (560 nm))
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** bei einer Konzentration von 0.064 mmol/l = 13.7 mg/l 20.7% Wachstumshemmung
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 37 Grad C; Ethanol als Loesevermittler (< 1 % v/v, nicht toxisch bei dieser Konzentration)
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (17)

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC11 :** = 2.7

**Method:** other: statischer Zellvermehrungshemmtest
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** nach 4 Stunden betrug die Hemmung 55 % im Vergleich zur unbehandelten Kontrolle
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 37 Grad C; Ethanol als Loesevermittler (keine Konzentrationsangabe, Kontrollen enthielten gleiche Menge Ethanol)
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (13)

**Species:** other fungi: Candida 107
**Exposure period:** 3 day(s)
**Unit:** g/l **Analytical monitoring:**
**EC0:** > 82.4

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 30 Grad C; geschuettelt
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (19)

**Species:** other fungi: Candida tropicalis
**Exposure period:** 1 day(s)
**Unit:** g/l **Analytical monitoring:**
**EC0:** > 82.4

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 30 Grad C; geschuettelt
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (19)

**Species:** other fungi: Saccharomyces carlsbergensis yeast
**Unit:** g/l **Analytical monitoring:**
**EC0:** > 82.4

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** 30 Grad C; geschuettelt; Glucose als Cosubstrat
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (19)

**Species:** other fungi: see remarks

**Method:** other: test for inhibition of spore germination
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Species: no antifungal activity up to:
Aspergillus niger 10000 mg/l (5 d; 28 degr. C; pH 5.6)
Trichoderma viride wood fungus 10000 mg/l ( " )
Trichophyton

Mentagrophytes soil fungus 1000 mg/l ( " )
Myrothecium verrucaria soil fungus? 10000 mg/l ( " )
Candida albicans 10000 mg/l (20 h; 37 degr. C; pH 5.6)
Mucor mucedo 10000 mg/l ( " )

**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

**Test condition:** petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l.

**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.

11-OCT-2005 (18)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)
**Unit:** µg/l **Analytical monitoring:** yes
**NOEC:** = 1.6 measured/nominal
**LOEC:** = 3.6 measured/nominal
**EC10 :** = 6.3 measured/nominal

**Method:** OECD Guide-line 211
**Year:** 2005
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 24.4, 68.6, 185.2 and 500 µg test item/L. Mean measured

concentrations of freshly prepared test solutions were <Limit of quantification, 9.9, 51, 138 and 367 µg/L The geometric means of mean measured initial and aged concentrations after 24 hours were <Limit of quantification, 1.6, 3.6, 13 and 77 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was withdrawn. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: Daphnia magna STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each Daphnia magna was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The Daphnia magna were fed at each renewal with suspensions of unicellular green algae. The suspensions of Desmodesmus subspicatus (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to
15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 20.4 to 21.4°C, the light intensity was in the

range 598 to 680 lux. The oxygen saturation never fell below 75 % (6.0 mg/L), and the mean pH was 9.3 to 9.4 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent Daphnia magna were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn Daphnia magna in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:
o Mortality (immobility) of parental generation Daphnia magna
o Age at first brood
o Total number of offspring per replicate
o Cumulative Number of live offspring per surviving female at the time of recording
o Intrinsic rate of increase, r
o Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-tetradecanol-d29 as internal standard. The method was validated for the determination of the test item in Daphnia test medium in the concentration range of 0.5 - 100 µg/L.

**Result:** SURVIVAL, GROWTH AND REPRODUCTION DATA

| Test item Nominal conc. (µg/L) | Survival (%) | Growth (length) Mean ± SD (mm) | Age at first brood Mean ± SD (days) |
|---|---|---|---|
| Control | 100 | 4.47 ± 0.32 | 7.8 ± 0.8 |
| 24.4 | 100 | 4.83 ± 0.31 | 7.7 ± 0.7 |
| 68.6 | 100 | 4.50 ± 0.38 | 8.1 ± 0.7 |
| 185.2 | 100 | 4.49 ± 0.27 | 8.2 ± 0.8 |
| 500 | 70 | 4.73 ± 0.40 | 7.9 ± 0.6 |

| Test item nominal conc. (µg/L) | Cumulative offspring per female Mean ± SD (#) | Intrinsic rate of increase r Mean ± SD (1/d) |
|---|---|---|
| Control | 86.6 ± 5.7 | 0.368 ± 0.032 |
| 24.4 | 84.0 ± 7.4 | 0.364 ± 0.034 |
| 68.6 | 79.7 ± 9.4 | 0.347 ± 0.033 |
| 185.2 | 73.9 ± 8.5 | 0.338 ± 0.035 |
| 500 | 70.4 ± 8.2 | 0.338 ± 0.024 |

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 70 µg test item/L
EC20 = 270 µg test item/L

LOEC = 51 µg test item/L
NOEC = 9.8 µg test item/L
Related to mean measured concentrations:
EC10 = 6.3 µg test item/L
EC20 = 23 µg test item/L
LOEC = 3.6 µg test item/L
NOEC = 1.6 µg test item/L

Test substance:
C14 Fatty alcohol (1-Tetradecanol)
CAS No. 112-72-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 30527
Purity: 99.5 % ± 0.5 %

**Test substance:** C10 Fatty alcohol (1-Decanol)
CAS No. 112-30-1
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 21011
Purity: 99.5 % ± 0.5 %

**Reliability:** (1) valid without restriction
Guideline study conducted in accordance with GLP.

**Flag:** Critical study for SIDS endpoint

04-NOV-2005 (62)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The

enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (15)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | other: COX-SD |
| **Sex:** | male/female |
| **No. of Animals:** | 10 |
| **Vehicle:** | other: 50% w/w suspension in 1% w/w gum tragacanth |
| **Doses:** | 7.26, 12.62, 15.89 and 20 g/kg |
| **Value:** | > 20000 mg/kg bw |
| **Method:** | other: contract laboratory protocol |
| **Year:** | 1977 |
| **GLP:** | no data |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY:<br>- Time of death: Observation days 5 (dose level 12.62 g/kg), 6 and 10 (dose level 20 g/kg).<br>- Number of deaths at each dose: 0/10, 1/10, 0/10, 2/10 all deaths were amongst females.<br><br>CLINICAL SIGNS: Animals at each dose displayed the following: hypoactivity, diarrhea, hypersalivation, diuresis, ocular porphyrin deposits, unthriftiness, thinness, and emaciation. Surviving animals returned to normal between 1 and 10 days following dosage. All survivors showed weight gains within expected limits by the end of the observation period.<br><br>NECROPSY FINDINGS: Two animals which succumbed had moderate to severe congestion of the kidneys, adrenals, liver, lungs, stomach and gastrointestinal tract, haemorrhages (1 rat), and erosion of the mucosa of the stomach. The remaining decedent was in an advanced state of autolysis and no conclusions could be drawn. Of the animals that were sacrificed, gross necropsy findings were unremarkable.<br><br>POTENTIAL TARGET ORGANS: Erosion of the gastric mucosa was noted in 2 decedents.<br><br>SEX-SPECIFIC DIFFERENCES: Females appear rather more susceptible, mortalities were confined to the females. |
| **Source:** | Scientific Associates, Inc. 1977b<br>Hayes Consultancy Service Bromley, Kent<br>Shell Chemicals Ltd. London<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: rat (COX-SD)<br>- Source: not reported<br>- Weight at study initiation: 210-299g<br>- Group size: 5M+5F fasted<br>- Controls: no |

ADMINISTRATION: Gavage
- Doses: 7.26, 12.62, 15.89 and 20 g/kg (based on range finder)
- Doses per time period: single
- Volume administered or concentration: 50% suspension highest practical dose 20 g/kg.
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for clinical signs of toxicity and death several times on the day of dosing and daily thereafter. All decedents and survivors were necropsied. Survivors were weighed at the end of the observation period.

**Test substance:** Tradename Alfol 14

**Conclusion:** The rat oral LD50 for Alfol 14 is >20 g/kg. Animals at all dose levels showed signs of intoxication following dosing these persisting from 1 to 10 days. Erosion of the gastric mucosa was observed in two decedents but not in survivors.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Well documented and conducted study.

**Flag:** Critical study for SIDS endpoint

16-JUL-2005 (64)

**Type:** LD50
**Species:** rat
**Strain:** other: Carworth-Wistar rat
**Sex:** male
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Doses:** not reported
**Value:** = 32500 ml/kg bw

**Method:** other: Smyth et al, 1962
**Year:** 1969
**GLP:** no
**Test substance:** other TS: Tetradecanol (mixed isomers)

**Result:** The rat oral LD50 for the mixed isomers of tetradecanol was 32.5 ml/kg (confidence limits 29.1 - 36.5). The density is not given in the publication but assuming a density of the order of 0.83 (from physical data included in this Iuclid) this gives an LD50 of 26.98 g/kg.

This value is also reported by Opdyke, 1975.

**Source:** Smyth et al. 1969

Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Carworth-Wistar)
- Age: 5 weeks
- Group size: 5/group non-fasted
- Controls: no

ADMINISTRATION:
- Doses: not reported
- Doses per time period: single
- Volume administered or concentration: undiluted

- Post dose observation period: 14 days

EXAMINATIONS: Mortality only. LD50 calculated using the methods of Weil (1952) and Thompson (1947).

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.

**Flag:** Critical study for SIDS endpoint

16-OCT-2004 (53) (54) (68)

**Remark:** Summary data reported in secondary references. Rat oral LD50 >5g/kg. Unpublished data Levenstein, 1972. No other details provided. This appears to be the same reference reported in Iuclid 2000 as Henkel unpublished report archive TBD 790109 (no. 232)

**Source:** Hayes Consultancy Service Bromley, Kent

**Test substance:** As prescribed.

**Reliability:** (4) not assignable
Secondary reference.

16-OCT-2004 (44) (53) (57)

**Remark:** Summary report, the LD50 in Holzman rats was reported as >8.0 g/kg. No further details available.

**Source:** Hayes Consultancy Service Bromley, Kent

**Test substance:** As prescribed.

**Reliability:** (4) not assignable
Secondary reference.

15-OCT-2004 (12)

## 5.1.2 Acute Inhalation Toxicity

**Type:** other: Inhalation
**Species:** rat
**Strain:** other: COX-SD
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: produced as a heated vapour
**Doses:** 1.5 mg/l
**Exposure time:** 1 hour(s)
**Value:** > 1.5 mg/l

**Method:** other: In house protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All rats survived the exposure period and subsequent 14 day observation period.

CLINICAL SIGNS: There were no signs of toxicity during the exposure period or the 14 day observation period. All rats gained in bodyweight at an expected rate over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported.

**Source:** Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Conclusion:** The rat 1 hour inhalational LC50 for Alfol 14 is >1.5 mg/l. There were no signs of toxicity and findings at gross necropsy were unremarkable.

**Test condition:** TEST ORGANISMS: Rat (COX-SD)
- Source: not reported.
- Weight at study initiation: 210-299g
- Number of animals: 5M+5F
- Controls: none

ADMINISTRATION: 1 hour, inhalation, whole body exposure.
- Type of exposure: the atmosphere was generated as a heated vapour, following exposure the animals were washed to remove any accumulated test material.
- Concentrations: 1.5 mg/l for 1 hour (not monitored)
- Particle size: vapour
- Type or preparation of particles: The vapour was generated by heating Alfol 14 in a water bath to 60C.
- Postexposure period: 14 days

EXAMINATIONS: The animals were observed frequently on the day of exposure and daily thereafter. Survivors were weighed and necropsied at the end of the exposure period.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

15-OCT-2004 (64)

**Type:** LC50
**Species:** rat
**Strain:** other: Carworth-Wistar
**Sex:** male/female
**No. of Animals:** 6
**Doses:** Saturated vapour concentration
**Exposure time:** 8 hour(s)

**Method:** other: Smyth et al, 1962
**Year:** 1969
**GLP:** no data
**Test substance:** other TS: tetradecanol (mixed isomers)

**Result:** All rats survived this 8 hour static exposure to the concentrated vapours. LC50 > saturated vapour concentration. Result also reported in secondary references Iuclid 2000, Opdyke, 1975, JACT, 1988.

**Source:** Smyth et al, 1969
Hayes Consultancy Service Bromley, Kent

**Test condition:** A group of 6 rats (sex unspecified) were exposed to concentrated vapours of the test substance for up to 8 hours using a static exposure technique.

**Reliability:** (4) not assignable
Screening test only, gives some indication of toxicity but exposure was static, methods described in an earlier

publication Smyth et al. Am. In. Hyg. Assoc. J. 23:95-107, 1962.

01-JAN-2005 (12) (44) (53) (68)

**Remark:** Secondary report of unpublished data, unobtainable. 10 young Sprague-Dawley rats (average weight 250 g) were exposed (whole body) to an aerosol containing 3% myristyl alcohol. The exposure consisted of intermittent bursts of 10 sec of aerosol, one every 3 minutes, total of 20 in the hour exposure. It was extimated that the average test substance concentration was ca 192 mg/l in air.

None of the exposed animals died. However, following 10 minutes exposure, ataxia and moderate nasal irritation were reported in all test animals persisting throughout the exposure period and for up to 4 hours after removal from the chamber.

**Source:** JACT, 1988
Hayes Consultancy Service Bromley, Kent

**Test substance:** Aerosol containing 3% myristyl alcohol (1-hexadecanol).

**Reliability:** (4) not assignable
Secondary reference.

16-JUL-2005 (12)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: 50% w/w dilution tetradecanol in 1 % w/w gum tragacanth
**Doses:** 2, 4 and 8 g/kg
**Value:** = 8000 mg/kg bw

**Method:** other: Contract laboratory protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: On observation days 9 and 11.
- Number of deaths at each dose: abraded 0/2, 0/2 and 2/2; intact 0/2, 0/2, 0/2.

LD50 M+F 8000 mg/kg It appeared that most of the test material remained unabsorbed on the skin.
APPLICATION SITE: At 24 hours after administration all animals showed slight to moderate erythema, desquamation, wrinkling and dryness. In all surviving animals desquamation and wrinkling persisted to the end of the observation period.

CLINICAL SIGNS: At 8000 mg/kg, two surviving animals showed signs of weakness, emaciation and pallor. All returned to normal within 4 days of exposure. Body weights of surviving animals showed a slight loss in 1 animal, constant weight in 1 animal and gains within expected limits in 8 animals.

NECROPSY FINDINGS: Animals which succumbed showed depleted visceral fatty tissue (1 rabbit), moderate dermal irritation, and desquamation at the treatment site (2 rabbits). One animal, which was sacrificed, showed a slight accumulation of clear, viscous fluid within the peritoneal cavity and crazing over the kidney cortex. In all other animals the necropsy findings were unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: not reported
- Weight at study initiation: 2.3-2.9 kg
- Group size: 2M+2F (1M+1F each intact and abraded)
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: 50% in 1% w/w gum tragacanth
- Total volume applied: maximum dose 3-4 ml/kg
- Doses: 2, 4 and 8 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

**Test substance:** Tradename Alfol 14

**Conclusion:** The rabbit dermal LD50 (24 hour occluded) for Alfol 14 was approx. 8000 mg/kg. All survivors showed skin irritation at the application site throughout the observation period. Signs of intoxication included weakness, emaciation and pallor.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

16-JUL-2005 (64)

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male
**Vehicle:** other: undiluted
**Value:** = 7.13 ml/kg bw

**Method:** other: Smyth et al, 1962
**Year:** 1969
**GLP:** no data
**Test substance:** other TS: tetradecanol (mixed isomers)

**Result:** Results were not reported in detail. The LC50 was 7.13 ml/kg (confidence limits 4.41-11.52 ml/kg). Equivalent to 5847 mg/kg using the density of 0.82 g/cm3, reported in chapter 2.3. No other details available.
**Source:** Smyth 1969
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: rabbit
- Source: no data
- Weight at study initiation: 2.5 -3.5 kg
- Group size: 4
- Controls: no

ADMINISTRATION: dermal
- Area covered: entire trunk
- Occlusion: Yes
- Vehicle: none
- Concentration in vehicle: undiluted

EXAMINATIONS: Clinical signs, 14 day observation period.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.
11-MAY-2006 (68)

**Remark:** Secondary report of unpublished data provided by Levenstein, 1974 (original unobtainable). The acute dermal LD50 in rabbits is reported as >5g/kg. This values also reported by RTECS, 2004, Iuclid 2000 and Patty 2001.
**Source:** Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
**Test substance:** As prescribed.
**Reliability:** (4) not assignable
Secondary reference.
16-OCT-2004 (44) (53) (54) (57)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** 50 %
**Exposure:** Occlusive

**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** other: 1% gum tragacanth
**PDII:** 4.3
**Result:** irritating
**EC classificat.:** irritating

**Method:** other: contract laboratory protocol
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hours
- Erythema: Intact skin 2.43, abraded skin 2.53 (72 hours score intact 2.4, abraded 2.8) Individual scores 5/6 greater than 2.3.
- Oedema: intact skin 1.83, abraded skin 3.26 (72 hours score intact 1.3, abraded 1.5)

REVERSIBILITY: Erythema increased or persisted until 72 hours after application while oedema decreased or persisted.

OTHER EFFECTS: None reported.

**Source:** Scientific Associates, 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour application to intact and abraded skin.
- Preparation of test substance: As a suspension.
- Area of exposure: 1 inch square
- Occlusion: Occlusive
- Vehicle: 1% gum tragacanth
- Concentration in vehicle: 50%
- Total volume applied: 1 ml (500 mg Alfol 14)
- Postexposure period: 72 hours
- Removal of test substance: Washed off the treated skin (no further details).

EXAMINATIONS
- Scoring system: Draize et al, 1944
- Examination time points: 24, 48 and 72 hours after application.

**Conclusion:** Based on the erythema and oedema scores reported Alfol 14 would be considered a skin irritant according to EU criteria and a class 2 irritant according to GHS criteria. Individual 24+48+72 hour erythema scores were >2.3 in 5/6 animals while the group mean 24+48+72 hour score was also in excess of 2.3 (2.46).

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

Well documented and conducted study.
**Flag:** Critical study for SIDS endpoint
16-JUL-2005 (64)

**Species:** human
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 20
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: patch test based on OECD 404
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test).
**Source:** Hayes Consultancy Service Bromley, Kent
**Test condition:** The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.
Study was performed under Good Clinical Practice (GCP).
**Test substance:** Tradename Lorol 14
**Conclusion:** Lorol C12-98 is not irritating to human skin following a 4 hour semi-occlusive exposure.
**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
**Flag:** Critical study for SIDS endpoint
25-OCT-2005 (25)

**Species:** human
**Concentration:** undiluted
**Exposure:** Open
**Exposure Time:** 1 hour(s)
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: open epicutaneous test according to Burckhardt
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Slight redness was observed after the 1 hour application period which disappeared within 15 minutes.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test condition:** The effect on human skin was investigated:
Undiluted test substance was applied to the forearm with a glass rod for a total application period of 60 minutes. Every 30 seconds, the test substance was gently swabbed with tissue and new test substance applied. Objective findings (erythema, edema) and subjective sensations (e.g. itching, cauterization etc.) were recorded after 15, 30, 45 and 60 minutes.
20 male and female volunteers of average age 35.3 years were

tested.

Study was performed under Good Clinical Practice (GCP).
**Test substance:** Tradename Lorol 14
**Conclusion:** Lorol C12-98 was essentially non-irritating to human skin following repeated application to non-occluded skin over a period of 1 hour.
**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
25-OCT-2005 (24)

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1974
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This monograph gives a brief report of a skin irritation study carried out with undiluted 1-tetradecanol using the Draize method with 24 hour occluded application to intact and abraded rabbits skin. The unpublished data was submitted by Levenstein 1974 and is also reported in Iuclid 2000 adn Patty, 2001.
**Result:** The undiluted C14 alcohol 1-tetradecanol was reported to be non-irritating to the skin following a 24 hour occluded exposure to intact and abraded rabbits skin. No further experimental details or irritation scores are available.
**Source:** Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44) (53) (54)

**Species:** human
**Concentration:** 12 %
**Exposure:** Occlusive
**Exposure Time:** 48 hour(s)
**Vehicle:** petrolatum
**Result:** not irritating

**Method:** other
**Year:** 1974
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This monograph gives a brief report of a skin irritation study carried out with undiluted 1-tetradecanol on human skin. 1-tetradecanol was tested against 2 panels of human subjects using a 48 hour closed patch test. This is a report of unpublised data provided by Kligman, 1974.
**Result:** 1-tetradecanol did not cause irritation to human skin

following a 48 hour closed-patch exposure.
**Source:** Opdyke, 1975
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (53)

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Open
**Exposure Time:** 24 hour(s)
**No. of Animals:** 5
**Result:** not irritating

**Method:** other: Smyth et al, 1962
**Year:** 1969
**GLP:** no data
**Test substance:** other TS: mixed isomers of tetradecanol

**Result:** The skin showed just perceptible capillary injection indicating minmal skin irritation.
**Source:** Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
**Test condition:** This is a non-standard test. The test material is applied for a 24 hour uncovered exposure in a volume of 0.01 ml of either the undiluted material or dilutions in water or solvent. For this test the material was applied undiluted.
**Reliability:** (3) invalid
Non standard method not comparable to modern guidelines.
25-OCT-2005 (53) (68)

**Species:** other: rabbit, guineapig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** other TS: even C6-22 alcohols

**Result:** The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings

together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible. This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparative study meeting generally accepted scientific principles.

25-OCT-2005 (44) (45)

**Remark:** Secondary reference by RTECS to data reported in Cutaneous Toxicity, proceedings of the 3rd Conference 1967. Drill & Lazar (eds). Academic Press, Inc. 1977. Not available.

Summary report indicates that 75 mg of the test substance was applied to human skin daily for 3 days producing a moderate skin reaction.

**Source:** RTECS, 2004
Hayes Consultancy Service Bromley, Kent

**Test substance:** Reported as 1-tetradecanol Cas # 112-72-1

**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (57)

**Remark:** Report of unpublished reports from Henkel KGaA, TBD 860374 and 860375, originals unavailable.

The test substance was applied daily to rabbit skin on 4 consecutive days. Scoring according to Draize. Weak to sight skin reactions were observed after the first application, these did not intensify with subsequent appllications. Reaction described as slightly irritation.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** As prescribed. Samples of Lorol 14 tested obtained from Fa. Leciva, Prague.
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44)

**Remark:** Secondary report of unpublished data from Henkel KGaA TBD 820011 and 820230 no 443. Original not available.

Test according to Directive 84/449/EEC, B4. Rabbit skin irritation described as slightly irritating, no further details provided.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** As prescribed.
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44)

**Remark:** Secondary report of a study in hairless mice, unpublished report from Henkel KGaA TBD 760109 no 232.

The test substance was applied twice daily to the mouse skin and gently massaged into the skin. The number of treatment days was not reported. No further details available.

Result: described as not irritating.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** As prescribed.
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44)

**Remark:** Secondary report of a study in hairless mice, unpublished report from Henkel KGaA TBD 7820011 and 820230 no 443.

Applied to the skin of hariless mice. No other details available.

Result: described as slightly irritating.
**Source:** Hayes Consultancy Service Bromley, Kent

**Test substance:** As prescribed.
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44)

**Remark:** Secondary report of unpublished data from Henkel KGaA R9601427. Original not available.

Application to human skin apparently to OECD guideline 404 was reported as being non-irritating. NO other details available.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** As prescribed.
**Reliability:** (4) not assignable
Secondary reference.
25-OCT-2005 (44)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** moderately irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: Individual scores 0, 1, 1 (group mean 0.7)
- Iris: individual scores 0, 1, 0.3 (group mean score 0.43)
- Conjunctivae (Redness): Individual scores 0.7, 2, 1.7 (group mean score 1.47)
- Conjunctivae (Chemosis): Individual scores 0.3, 1.7, 1.7 (group mean score 1.23)
- Overall irritation score: Maximum group mean score 27.3 at 24 hours.

The substance is classified as a moderate irritant according to Kay and Callandra.

DESCRIPTION OF LESIONS: Diffuse corneal opacity was noted in 2 treated eyes at the 24, 48, and 72 hour observations. Iridial inflammation was noted in 2 treated eyes at the 24 hour observation and persisted in 1 treated eye at the 48 and 72 hour observations.
Moderate conjunctival irritation was noted in all treated eyes 1 hour after treatment and persisted in 2 treated eyes at the 24 and 48 hour observations. Minimal conjunctival irritation was noted in 1 treated eye at the 24 and 48 hour observations and in 2 treated eyes at the 72 hour and 7 day observation.

REVERSIBILITY: All corneal and iridial scores and scores for

conjunctival chemosis were normal by day 7. Conjunctival redness persisted in 2 rabbits through day 7 but scores were 0 by day 14. The effects were therefore fully reversible.

OTHER EFFECTS: Discharge was observed from all treated eyes 1 hour after instillation and persisted in one eye for 48 hours and in another for 72 hours. All eyes were clear at 7 days.

**Source:** Sanders 1996f
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.67-2.94 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and was ground to a fine powder prior to instillation. Measured using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 46 mg)
- Vehicle: None
- Postexposure period: 14 days

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 14 days
- Tool used to assess score: Standard ophthalmoscope.

**Test substance:** Tradename Kalcol 4098.

**Conclusion:** Kalcol 4098 applied as a powder is not classifiable as an eye irritant according to EU criteria. Kalcol 4098 is however a category 2A eye irritant according to GHS criteria based on corneal opacity of >= 1 in 2 test animals and persistence beyond 7 days. Effects were fully reversible by day 14.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

16-OCT-2004 (60)

**Species:** other: New Zealand White rabbit
**Concentration:** 10 %
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** other: polyethylene glycol 400
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0

- Conjunctivae (Redness): Individual scores 0.3, 0.3, 0 (group mean score 0.2)
- Conjunctivae (Chemosis): 0. 0, 0.3 (group mean score 0.1)
- Overall irritation score: maximum group mean score 8.7 at 1 hour post instillation. Described as a minimal eye irritant according to modified Kay & Calandra.

DESCRIPTION OF LESIONS: At 1 hour post instillation Grade 2 redness of the conjunctival membrane was noted in 2 treated eyes with grade 1 redness of the conjunctival membrane noted in the remaining treated eye. Conjunctival redness (grade 1) persisted in in 2 treated eyes at the 24 hour observation. Chemosis was also observed in all eyes at 1 hour post instillation (grade1 and 2) persisting in one treaed eye until 24 hours. Grade 3 discharge was noted in 1 treated eye with grade 1 noted in one other treated eye at the 1 hour observation. No other evidence of eye irritation was noted during the study.

REVERSIBILITY: All treated eyes appeared normal 48 and 72 hours after instillation.

OTHER EFFECTS:

**Source:** Hempstock 1997b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.56-2.80 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was prepared as a 10% solution in polyethylene glycol 400,
- Amount of substance instilled: 0.1 ml
- Vehicle: polyethylene glycol 400
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Calandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

**Test substance:** Tradename Kalcol 4098.

**Conclusion:** When instilled into the rabbit eye as a 10% solution in polyethylene glycol 400, Kalcol 4098 was not classified as an eye irritant by either EU of GHS criteria.

**Reliability:** (1) valid without restriction
Guideline study.

16-OCT-2004 (23)

**Species:** rabbit
**Concentration:** 100 mg
**Exposure Time:** 24 hour(s)
**Comment:** rinsed after (see exposure time)

**No. of Animals:** 6
**Vehicle:** other: applied as solid
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: contract laboratory protocol
**Year:** 1997
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE: The scores were reported as prescribed by the FDA 1965. Although individual animal data was provided only the converted scores were reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each time point was as follows:

1 hour: 6.7
24 hours: 18
48 hours: 12.5
72 hours: 6

DESCRIPTION OF LESIONS:
- Cornea: opacity slight to easily discernible involving 1/4 to 3/4 of the corneal surface observed in all animals. At 72 hours there was no corneal involvement in any animal.
- Iris: barely perceptible to minimal iritis (grade 1) in 1/6 rabbits at 24 hours after instillation. No iritis at 48 or 72 hours.
- Conjunctivae (Redness): Slight to moderate conjuctivitis in all eyes from 24 hours. At 72 hours there was minimal to slight redness in 6/6.
- Conjunctivae (Chemosis): Minimal to pronounced chemosis of the eye lids with a slight watery-mucoid discharge in all animals. At 72 hours barely perceptible to moderate chemosis 4/6 and slight discharge 2/6.

REVERSIBILITY: There was a gradual improvement in all animals. By the end of the 72 hour observation period there was no involvement of the iris or cornea. Minimal to slight redness and barely perceptible to moderate chemosis were still evident.

**Source:** Scientific Associates, Inc. 1977b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: The other eye served as control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: applied as a solid
- Amount of substance instilled: 100 mg
- Vehicle: none
- Postexposure period: 72 hours

- Rinsing: The treated eyes were rinsed after 24 hours to remove residual test material.

EXAMINATIONS
- Ophthalmoscopic examination: Not reported
- Scoring system: FDA 1965
- Observation period: 1, 24, 48 and 72 hours.
- Tool used to assess score: Fluorescein

**Test substance:** Tradename Alfol 14.
**Conclusion:** Based on the description of the lesions and the consistent reduction of severity of the effects over the 72 hours observation period it is considered that Alfol 14 is not classifiable as an eye irritant according to EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
12-OCT-2005 (64)

**Species:** rabbit
**Concentration:** 50 %
**No. of Animals:** 2
**Vehicle:** no data
**Result:** slightly irritating

**Method:** other: not specified
**GLP:** no
**Test substance:** other TS: C14 myristic alcohol

**Remark:** Summary report of unpublished Henkel data (Potokar Archive No. 232). No details of method except that 50 ul of 50% myristic alcohol was instilled. Slight conjunctival redness was reported up to 6 hours after instillation. There was no involvement of cornea or iris. Irritant response described as slight.

There is an entry in Iuclid 2000 describing slight eye irritation using the Draize method, this appears to be the same study as above as it refers to the same Henkel report.
**Source:** Iuclid 2000, Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference.
16-JUL-2005 (44)

**Remark:** This eye irritation test is based on a protocol developed in 1946 (Smyth & Carpenter, 1946). This involves instillation of various volumes and concentrations into the eye and is not a valid test method. The result given was grade 1 which equates to at most a very small area of necrosis resulting from instillation of 0.5 ml undiluted chemical.

The result is reported by RTECS, 2004 and Opdyke, 1975.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** Tetradecanol (mixed isomers)
**Reliability:** (3) invalid

Non-standard protocol not comparable to modern guidelines.
12-OCT-2005 (53) (57) (68)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** other: Hartley albino guinea pigs
**Concentration 1st:** Induction 5 % intracutaneous
**2nd:** Induction 50 % occlusive epicutaneous
**3rd:** Challenge occlusive epicutaneous
**No. of Animals:** 10
**Vehicle:** other: liquid paraffin
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** OECD Guide-line 406 "Skin Sensitization"
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: Following intradermal injection skin irritation was seen at concentrations of 10% and 5% persisting for 72 hours but less marked at the lower concentration. The 3% concentration showed evidence of irritation at 24 hours in one animal only. Loweer concentrations from 0.1 -1% showed no irritation. Following topical application slight irritation was seen in 2/4 animals at 50% only.

RESULTS OF TEST
- Sensitization reaction: There was no evidence of sensitisation in any of the test or control animals at either challenge concentration. Response 0/10 test, 0/5 control.
- Clinical signs: There were no significant differences in general condition and body weight gain between test and control groups over the course of the test.
- Rechallenge: Not required.

**Source:** Iihama 1997b
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pigs
- Strain: albino Hartley
- Sex: female
- Source: Japan SLC, Shizuoka
- Age: 4 weeks
- Weight at study initiation: 276-323 g
- Number of animals: 10F
- Controls: 5F

ADMINISTRATION/EXPOSURE
- Study type: adjuvant, maximization test
- Preparation of test substance for induction: In liquid paraffin
- Preparation of test substance for induction: In liquid paraffin
- Induction schedule: Single intradermal injection followed 7 days later by a 48 hour occlusive patch applied topically.
- Concentrations used for induction: 5% intracutaneous, 50%

topical
- Concentration in Freuds Complete Adjuvant (FCA): 1:1 water in oil emulsion of 10% test substance in FCA and saline.
- Challenge schedule: 21 days after first induction topical application of an occluded patch for 24 hours.
- Concentrations used for challenge: 3 and 10%
- Rechallenge: No
- Positive control: DNCB and formalin, not concurrent, evidence presented over a relevant time period that the strain of guinea pig did respond to known sensitisers.

EXAMINATIONS
- Grading system: 0 = no visible change, 1 = discrete or patch erythema; 2 = moderate and confluent erythema; 3 = intense erythema and swelling.
- Pilot study: Using 4 animals and multiple patches Kalcol 4098 was tested at concentrations from 0.1% - 10% intradermally and at 3, 10, and 50% topically.

**Test substance:** Tradename Kalcol 4098.
**Conclusion:** Kalcol 4098 is not a skin sensitiser when tested according to the M&K maximisation procedure.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
05-DEC-2005 (42)

**Type:** other: human maximisation test
**Species:** human
**No. of Animals:** 50
**Vehicle:** petrolatum
**Result:** not sensitizing

**Method:** other: human maximisation test
**Year:** 1974
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Tetradecanol at a concentration of 12% in petrolatum was tested in two series of 25 human volunteers using the numan maximisation procedure of Kligman 1966 and Kligman & Epstein, 1975. In the first panel sensitisation reactions were reported in 2/25 volunteers. No sensitisation reactions were observed in the second test panel. Overall it appears that tetradecanol is not a skin senisiter in man.

Secondary reference report of unpublished data from Kligman 1974.
**Source:** Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference.
16-JUL-2005 (53)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-acute
**Species:** rat **Sex:** male
**Strain:** Wistar
**Route of administration:** oral feed

**Exposure period:** 12 days
**Control Group:** yes, concurrent no treatment

**Method:** other
**Year:** 1971
**GLP:** no
**Test substance:** other TS: described as myristyl alcohol no detail of purity or isomeric content.

**Remark:** This study was undertaken to evaluate the available energy provided by myristyl alcohol and other alcohols, acids, esters and carbonyl substances in the diet. Myristyl alcohol at a concentration of 5% and 10% in the diet was administered over a 12 day period to 8 rats. All rats administered myristyl alcohol in the diet at 10% died within the 12 days. 2/8 rats receiving dietary myristyl alcohol at 5% also died.

Cited by Opdyke, 1975
**Source:** Hayes Consultancy Service Bromley, Kent
**Reliability:** (3) invalid
As many of the rats died little information can be drawn from this study.
25-JAN-2005 (53) (85)

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for tetradecanol, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A) and C16 (1-hexadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (66) (78)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Bacterial reverse mutation assay
**System of testing:** Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
**Concentration:** Test 1: 15 - 5000 ug/plate; Test 2: 50 to 5000 ug/plate
**Cytotoxic Concentration:** >5000 ug/plate

**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: 1500 ug/plate, plates were counted manually at this concentration and above.

CYTOTOXIC CONCENTRATION: Slight cytotoxicity was indicated in a preliminary toxicity screen with TA100 at dose levels >= 500 ug/plate without metabolic activation. In the actual mutation study there was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.

**Source:** Thompson 1996b.

Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced

ADMINISTRATION:
- Dosing: Test 1: 15 (-S9 only), 50, 150, 500, 1500 and 5000 ug/plate. Test 2: 50, 150, 500, 1500 and 5000 ug/plate.
- Number of replicates: triplicate
- Application: Plate incorporation assay, vehicle DMSO
- Positive and negative control groups and treatment: Vehicle control- DMSO. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to controls.

**Test substance:** Tradename Kalcol 4098.
**Conclusion:** The C14 alcohol Kahlcol 4098 did not increase the reverse mutation rate in histidine dependent bacterial strains of

Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

16-OCT-2004 (74)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol, dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Source:** Hayes Consultancy Service Bromley, Kent

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (43) (66) (67) (78)

## 5.7 Carcinogenicity

**Species:** mouse **Sex:** female
**Strain:** Swiss
**Route of administration:** dermal
**Exposure period:** 60 weeks
**Frequency of treatment:** three times weekly
**Post exposure period:** none
**Doses:** 4 ug/mouse in cyclohexane
**Result:** negative
**Control Group:** no

**Method:** other: skin tumour promotion study
**Year:** 1966
**GLP:** no data
**Test substance:** other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.

**Source:** Sice 1966.

Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane
- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)
- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Test substance:** The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Conclusion:** In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour

development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999).

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment however irritaton at the application site is a confounder.

16-OCT-2004 (8) (44) (50) (51) (53) (57) (65)

**Species:** mouse **Sex:** no data
**Strain:** other: Swiss albino ddY
**Route of administration:** i.p.
**Exposure period:** 5 days
**Frequency of treatment:** daily
**Post exposure period:** 24 days
**Doses:** Test 1: 2.5 or 10 mg/mouse/day. Test 2: 2, 4 or 8 mg/mouse/day 2.5 and 10 mg/mouse/day for C16 & 18 alcohols.
**Result:** negative
**Control Group:** yes

**Method:** other: determination of antitumour activity against Ehrlichs Ascites Tumour
**Year:** 1972
**GLP:** no
**Test substance:** other TS: Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** The C10, 12, and 14 alcohols exhibited toxicity to the mice, evidenced by severe diarrhoea and loss of body weight. The dose levels were reduced in the repeat test. The mean survival time for the untreated control group (Ascites implantation only) was 18.3 days in test1 and 14.4 days in test 2. All of the alkanols tested increased the survival time of mice implanted with ascites tumour cells at one or more dose levels tested. Life span was prolonged by 124 - >194%.
**Source:** Ando et al, 1972
Hayes Consultancy Service Bromley, Kent
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS Mouse Swiss albino ddY implanted ip with ascites tumour cells.
- Age: 5 weeks
- Weight at study initiation: 20-23g
- Number of animals: 4 or 6/ treatment group, 20 controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 5 days starting 24 hours afeter implantation of the ascites tumour cells.
- Type of exposure: Intraperitoneal
- Post exposure period: 24 days
- Vehicle: Probably aqueous suspension using Tween 80.
- Concentration in vehicle: Not reported.
- Doses: Test 1: for all 5 alcohols tested dose levels were 2.5 and 10 mg/mouse. Test 2: C10, 12 and 14 alcohols were tested at 2, 4 and 8 mg/mouse, C16 and 18 alcohols were tested at 2.5 and 10 mg/mouse.

OBSERVATIONS
The mean survival time was recorded and compared to the untreated control group.

**Conclusion:** Treatment with C10 -18 alcohols extended the survival time of mice implanted intraperitoneally with Ehrlich ascites tumour cells.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
16-OCT-2004 (2) (53)

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C14 alcohol (tetradecanol) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol) and from the supporting substance C18 (octadecanol).
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (66) (67) (78)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that tetradecanol is not expected to be a developmental toxicant in the absence of maternal toxicity.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for

assessment.

15-SEP-2005 (66) (67) (78)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: allergic skin reaction in man

**Remark:** In a retrospective survey of allergic reactions to cosmetics, data on 475 patients with contact allergy to cosmetic ingredients were collected in 5 European dermatology centres. The observations were made over a 4 month period in 1996. A positive response to myristyl alcohol was obtained in only 1/475 patients.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** Myristyl alcohol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

25-JAN-2005 (20)

**Type:** other: allergic skin reaction in man

**Remark:** The authors report the results of patch testing with aliphatic alcohols in 1664 consecutive patients at a dermatological clinic. Patch testing with myristyl alcohol, 5% in vaseline, resulted in 9 positive reactions (incidence 0.5%) while 10% vaseline produced 21 positive reactions (1.3%)

Cited in the Cosmetic Ingredient Review, 1988.
**Source:** Hayes Consultancy Service Bromley, Kent
**Test substance:** Myristyl alcohol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

26-JAN-2005 (39)

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 629-76-5
**CAS No.** 629-76-5
**EINECS Name** pentadecan-1-ol
**EC No.** 211-107-9
**Molecular Formula** C15H32O

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
**Revision date:**
**Date of last Update:** **28-DEC-2005**

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**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
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**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
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**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom

03-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
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**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
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**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
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**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano
**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
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**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
03-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Pentadecanol
**Smiles Code:** OCCCCCCCCCCCCCCC
**Mol. Formula:** C15 H32 O1
**Mol. Weight:** 228.42

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-pentadecanol, CAS 629-76-5 are >80% linear.

The substance comprises >90% C15, <10% C14. Components of even and odd chain length, in the range C14-15 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Pentadecanol (7CI, 8CI, 9CI) (CA INDEX NAME)
Pentadecanol (6CI)
Alfol 15
n-1-Pentadecanol
n-Pentadecanol
NSC 66446
Pentadecyl alcohol
Pentadecan-1-ol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are

considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-pentadecanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (6) (15) (24)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

## 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-pentadecanol. There could also be exposure from private use (for consumer

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

11-AUG-2003

## 2.1 Melting Point

**Value:** = 45 - 46 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (22)

**Value:** = 44 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment
04-JAN-2005 (14)

## 2.2 Boiling Point

**Value:** = 318 degree C

**Method:** other: (calculated) SRC MPBPVP v1.40
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The presence of branched components in the substance, within the limits described in section 1.1-1.4, is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely.

Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-SEP-2005 (1)

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (21)

### 2.3.1 Granulometry

-

### 2.4 Vapour Pressure

**Value:** = .0000512 hPa at 25 degree C

**Method:** other (measured)
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** PhysProp database
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of vapour pressure data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (9)

### 2.5 Partition Coefficient

**log Pow:** = 6.43 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The presence of branched components is not expected to significantly affect the predicted value.
Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

### 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .102 mg/l

**Method:** other: measured
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for water solubility values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (26)

**Solubility in:** Water
**Value:** = .0061 mg/l at 20 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
04-JAN-2005 (13)

**Solubility in:** Water
**Value:** = .103 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
04-JAN-2005 (7) (22)

**Solubility in:** Water
**Value:** = .093 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.093 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
11-SEP-2005 (1)

## 2.6.2 Surface Tension

-

**2.7 Flash Point**

-

**2.8 Auto Flammability**

-

**2.9 Flammability**

-

**2.10 Explosive Properties**

-

**2.11 Oxidizing Properties**

-

**2.12 Dissociation Constant**

-

**2.13 Viscosity**

-

**2.14 Additional Remarks**

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 22.43355E-12 cm3/molecule.sec
Half-life: 17.2 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
10-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

**Method:** The EU samples were obtained during 2001-2 from municipal waste water treatment plants. Each was obtained over a 24-hour period, and preserved by addition of formalin at the time of sampling.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivatisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Samples from Canada were grab samples obtained during August 2003, and were preserved with formalin.

**Remark:** The study is of effluent monitoring of 20 biofilm and activated sludge wastewater treatment plants from Europe (12) and Canada (8) receiving predominantly municipal effluent. Concentrations of alcohols and alcohol ethoxylates were measured.

**Result:** In the results, Provinces are indicated as 2-letter abbreviations. Results are presented as µg/L concentrations as:

| Location: Treatment Type | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Vernon, BC: TF | 0.393 | 0.174 | 0.428 | 0.886 | 0.452 | 0.718 | 3.051 |
| Kelowna, BC: AS | 0.243 | 0.102 | 0.107 | 0.181 | 0.095 | 0.121 | 0.849 |
| Toronto, ON: AS | 0.027 | 0.235 | 0.548 | 0.312 | 0.883 | 0.492 | 2.497 |
| La Prairie, QC: AS | 0.070 | 0.030 | 0.029 | 0.041 | 0.057 | 0.068 | 0.295 |
| Victoriaville, QC: AS | 0.069 | 0.019 | 0.014 | 0.048 | 0.026 | 0.109 | 0.285 |
| Paris, ON, AS | 0.036 | 0.030 | 0.033 | 0.059 | 0.083 | 0.060 | 0.301 |
| Cardston, AB: RBC | 1.251 | 0.961 | 3.354 | 3.257 | 3.180 | 2.174 | 14.2 |
| Waterloo, ON: AS | 0.301 | 0.122 | 0.156 | 0.172 | 0.160 | 0.127 | 1.038 |

TF = trickling filter
AS = activated sludge
RBC = rotating biological contactor

Data from activated sludge plants in Europe:

Total alcohol µg/L

| Location | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Northwich, UK | 0.468 | 0.319 | 0.305 | 0.154 | 0.485 | 0.591 | 2.322 |
| Cannock, UK | 0.104 | 0.087 | 0.069 | 0.084 | 0.179 | 0.318 | 0.841 |
| Rushmoor, UK | 0.134 | 0.104 | 0.095 | 0.125 | 0.338 | 0.408 | 1.204 |
| Kralingse Veer, NL | 0.410 | 0.147 | 0.138 | 0.125 | 0.368 | 0.138 | 1.326 |
| De Meern, NL | 0.282 | 0.208 | 0.174 | 0.155 | 0.472 | 0.239 | 1.53 |
| Horstermeer, NL | 0.360 | 0.211 | 0.212 | 0.136 | 0.598 | 1.209 | 2.726 |
| Estepona, ES | 0.214 | 0.073 | 0.182 | 0.148 | 0.999 | 1.144 | 2.76 |
| La Vibora, ES | 1.179 | 0.533 | 1.741 | 1.181 | 4.172 | 2.426 | 11.23 |
| Munich, DE | 0.010 | 0.023 | 0.007 | 0.034 | 0.005 | 0.008 | 0.087 |
| Torino, IT | 0.070 | 0.094 | 0.057 | 0.058 | 0.419 | 0.038 | 0.736 |
| Robecco, IT | 0.092 | 0.130 | 0.072 | 0.206 | 0.187 | 0.266 | 0.953 |
| Ratingen, DE | 0.046 | 0.052 | 0.033 | 0.083 | 0.037 | 0.068 | 0.319 |

(usual country and US state designators)
Results for all carbon numbers are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP monitoring studies conducted to a high standard.

21-DEC-2005 (8)

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 228.4
Data temperature 25 deg C
Log Kow 6.43
Water Solubility 0.102 mg/l
Vapour pressure 0.00512 Pa
Melting point 45 deg C
half life in air 17.2 h
half life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 0.10% |
| Soil | 97.6% |
| Water | 0.04% |
| Fish | 5.51E-03% |
| Sediment | 2.17% |

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 21.1 | 0.00128 | 1.12E-05 |
| % in water | 1.47 | 3.32 | 0.0107 |
| % in sediment | 42.7 | 96.7 | 0.31 |
| % in soil | 34.7 | 0.00211 | 99.7 |

The results reflect that the ultimate fate of 1-pentadecanol is dependent on its route of release into the environment.1-Pentadecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.In water, the adsorption coefficient of 1-pentadecanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (4)

## 3.3.2 Distribution

**Method:** Measurement of the sorption of five alcohols onto a mixture of activated sludge and river water suspended solids.
River water was collected from River Gowy, Ellesmere Port, on two successive days and mixed then sterilised. It contained 12

mg/L suspended solids.

Activated sludge was obtained from a municipal waste water treatment plant. The mixed liquor suspended solids content was determined to be 2940 mg/L. Total organic carbon was 880 mg/L. The mixture was sterilised, allowed to settle, and a simulated effluent was prepared to give 30 mg/L suspended solids. The fraction of organic carbon was 0.167. The vessel was spiked with TS to give ca. 100 µg/L. The test system was stirred for 24 h, which was sufficient to give equilibrium.

The mixed settled activated sludge with river water with up to 72 h equilibration.

**Remark:** The results for five substances are considered alongside each other since the results of the whole study are useful for comparison purposes.
The data for the alcohol ethoxylates obtained in the study do not need to be included in this summary.

**Result:** Alcohol sorption coefficients showed some time dependence, reaching a plateau by 72 h. C15 was found to be an unexplained outlier. The 72 h results were:

| C | 12 | 14 | 15 | 16 | 18 |
|---|---|---|---|---|---|
| Kd | 3000± 80 | 8490± 920 | 3080± 270 | 23800 ±3200 | 78700 ±5400 |
| Koc | 17980 | 50830 | - | 143000 | 471000 |
| log Koc | 4.25 | 4.71 | - | 5.15 | 5.67 |

These data (neglecting the C15) can be interpreted as a QSAR in the usual way as:

Log Koc = 0.11 + 0.77 log Kow

R2 = 0.994

The result is in line with typical QSARs of this type.

**Test substance:** Linear alcohols labelled with 14-C, radiochemical purity 99%

**Reliability:** (2) valid with restrictions
Although not a SIDS end point, this study is considered to be the best study of Koc for these carbon numbers.

21-DEC-2005 (16)

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The estimated log Kow value of 6.43 was used in the TGD calculation methods.

**Result:** TGD hydrophobics method: Koc = 203000
TGD Non-hydrophobics method: Koc = 23100
TGD Alcohols method: Koc = 1020
SRC PCKOCWIN method: Koc = 2050

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

**Method:** Laboratory continuous activated sludge study.

4 mg/L of TS
20°C
Hydraulic residence time (HRT) 6 h
Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples

were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.

**Remark:** This paper describes mainly the properties of alcohol ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.

**Result:** Results are corrected for control values.

| Alcohol | Conc. in effluent ng/L | Conc. in sludge µg/g | %removal |
|---|---|---|---|
| C12 | 18 | 0.6 | 98.6 |
| C13 | 21 | 0.7 | 99.5 |
| C14 | 5.5 | 0 | 99.6 |
| C15 | 2.9 | 1.1 | 99.8 |
| C16 | 1.6 | 0.01 | 99.5 |
| C18 | 58 | 0.7 | 99.1 |
| Total | 130 | 2 | 99.4 |

| | |
|---|---|
| Total elimination of ethoxylates | 97.4 |
| Total in waste sludge solids | 2.0 |
| Total in suspended solids | 0 |

This shows that most of that which does not degrade (itself a small amount) is in the solids.

**Test substance:** 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

| C | Mol ratio |
|---|---|
| 12 | 1 |
| 13 | 2 |
| 14 | 2.3 |
| 15 | 1.8 |
| 16 | 1.1 |
| 18 | 2.9 |

**Reliability:** (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

21-DEC-2005 (23)

**Method:** Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation

Liquid-chromatography-mass spectrometric (LCMS) technique.

**Result:** Influent (In), effluent (Eff) values in ug/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

| | | C12-15 OH | | | C16-18 OH | | |
|---|---|---|---|---|---|---|---|
| | WWTP type | In | eff | % | in | eff | % |
| TX | Lagoon | 297 | 2 | 99.3 | 92.7 | 2.4 | 97.4 |
| NJ | Oxidation Ditch | 249 | 0.7 | 99.7 | 181 | 0.8 | 99.6 |
| OH | Rotating biological contactor | 157 | 0.1 | 0.06 | 77 | 0.07 | 99.9 |
| IA | Trickling filter | 499 | 2.0 | 99.6 | 354 | 2.3 | 99.4 |
| MO | Trickling filter | 532 | 4.9 | 99.1 | 315 | 9 | 97.3 |
| KS | Lagoon | 67.5 | 1.1 | 98.4 | 35.4 | 2.2 | 93.8 |
| CA | Activated sludge | 20.05 | 0.2 | 99.9 | 169 | 0.4 | 99.8 |
| OR | Activated sludge | 92.9 | 0.2 | 99.8 | 133 | 0.6 | 99.5 |
| AZ | Oxidation ditch | 702 | 0.3 | 100 | 394 | 0.5 | 99.9 |

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP studies conducted to a high standard.

21-DEC-2005 (17)

## 3.6 BOD5, COD or BOD5/COD Ratio

**-**

## 3.7 Bioaccumulation

**BCF:** = 42600

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation

was used. This approach is in accordance with standard EU recommendations.

The estimated log Kow value of 6.43 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 1.56

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
The MIC concentration appears to be above the SPARC estimated water solubility of Pentadecanol.
**Source:** Hattori 1987.
**Reliability:** (3) invalid

Study was considered invalid due to significant methodological deficiencies.

17-OCT-2005 (11)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 23 day(s)
**Unit:** µg/l **Analytical monitoring:** yes
**NOEC:** = 7.8 measured/nominal
**LOEC:** = 19 measured/nominal
**EC10 :** = 62 measured/nominal

**Method:** OECD Guide-line 211
**Year:** 2005
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 30, 65, 139 and 300 µg test item/L. Mean measured concentrations of the freshly prepared test solutions were <Limit of quantification, 15, 56, 104 and 241 µg/L. The geometric means of mean measured initial and aged concentrations after 24 hours were <Limit of quantification, 2.0, 7.8, 19 and 63 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL

was withdrawn. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. The daphnia were exposed for 23 days (as opposed to the normal 21 days) in order to meet the criterion for reproduction. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: Daphnia magna STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each Daphnia magna was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The Daphnia magna were fed at each renewal with suspensions of unicellular green algae. The suspensions of Desmodesmus subspicatus (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to
15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 20.7 to 21.8°C, the light intensity was in the range 568 to 659 lux. The oxygen saturation was in the range 66 to 103% (the lowest concentration was equivalent to 5.4 mg/L), and the mean pH was 9.2 to 9.4 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent Daphnia magna were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn Daphnia magna in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated

quantitatively:
o Mortality (immobility) of parental generation Daphnia magna
o Age at first brood
o Total number of offspring per replicate
o Cumulative Number of live offspring per surviving female at the time of recording
o Intrinsic rate of increase, r
o Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using deuterated n-pentadecanol-d31 as internal standard. The method was validated for the determination of the test item in Daphnia test medium in the concentration range of 0.2 - 200 µg/L.

**Result:** SURVIVAL, GROWTH AND REPRODUCTION DATA

| Test item Nominal conc. (µg/L) | Survival (%) | Growth (length) Mean ± SD (mm) | Age at first brood Mean ± SD (days) |
|---|---|---|---|
| Control | 100 | 3.80 ± 0.34 | 9.0 ± 0.82 |
| 30 | 100 | 3.79 ± 0.28 | 9.0 ± 0.82 |
| 65 | 100 | 3.62 ± 0.33 | 9.3 ± 1.06 |
| 139 | 100 | 3.77 ± 0.52 | 9.2 ± 1.14 |
| 300 | 100 | 3.87 ± 0.19 | 8.9 ± 0.99 |

| Test item nominal conc. (µg/L) | Cumulative offspring per female Mean ± SD (#) | Intrinsic rate of increase r Mean ± SD (1/d) |
|---|---|---|
| Control | 63.4 ± 4.8 | 0.272 ± 0.010 |
| 30 | 60.7 ± 4.9 | 0.267 ± 0.018 |
| 65 | 59.3 ± 6.9 | 0.262 ± 0.013 |
| 139 | 54.8 ± 7.1 | 0.257 ± 0.018 |
| 300 | 50.8 ± 6.7 | 0.256 ± 0.020 |

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 74 (Confidence interval 7-130) µg test item/L
EC20 = 240 (Confidence interval 140-2200) µg test item/L
LOEC = 100 µg test item/L
NOEC = 56 µg test item/L

Related to mean measured concentrations:
EC10 = 12 (Confidence interval 2-23) µg test item/L
EC20 = 62 (Confidence interval 33-350) µg test item/L
LOEC = 19 µg test item/L
NOEC = 7.8 µg test item/L

**Test substance:** C15 Fatty alcohol (1-Pentadecanol)
CAS No. 629-76-5
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.

Lot No: 30527
Purity: 99.5 % ± 0.5 %

**Reliability:** (1) valid without restriction
Guideline study conducted in accordance with GLP.

**Flag:** Critical study for SIDS endpoint

04-NOV-2005 (18)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It

has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (10)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

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## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers and data for C14-15 and C14-16 alcohols. This data supports the statement that Pentadecanol is expected to be of low acute oral toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (25)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C13 (tridecanol Cas 112-70-9), C12-16 and C14 (tetradecanol) alcohols in support of the statement that C15 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (25)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers and data for C14-15 and C14-16 alcohols. This data supports the statement that Pentadecanol is expected to be of

low acute dermal toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (25)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. For the subcategory of essentially linear alcohols, of which Pentadecanol is a member, the skin irritation potential for the higher members in the range C12 - C16 is mild - essentially non-irritant. This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, together with data on C12-16, C14-15 and C14-16 alcohols. This supports the conclusion that Pentadecanol is expected to be mildly irritating to the skin.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Pentadecanol is expected to be mildly irritating to the skin.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (25)

## 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants while alcohols of chain length >C12 are essentially non-irritating to the eye. Data available for C12-15, C12-16, C14-15 and C14-16 alcohols support the conclusion that pentadecanol is expected to be essentially non-irritating to the eye.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Pentadecanol is expected to be essentially non- irritating to the eye.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (25)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12-16 (Type A), C14 (tetradecanol) and C16 (hexadecanol) alcohols which support the conclusion that Pentadecanol is not expected to be a skin sensitiser.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (25)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for pentadecanol, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A) and C16 (1-hexadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (25)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for pentadecanol is available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16

(types A&B), tetradecanol, hexadecanol and octadecanol [Ames].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (25)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol and hexadecanol [Ames].

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (12) (19) (20) (25)

## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C15 alcohol (pentadecanol) is not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the

reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A) and C16 (hexadecanol).
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (19) (20) (25)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that pentadecanol is not expected to be a developmental toxicant in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (19) (20) (25)

### 5.8.3 Toxicity to Reproduction, Other Studies

-

### 5.9 Specific Investigations

-

### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

-

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(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 36653-82-4 |
| **CAS No.** | 36653-82-4 |
| **EINECS Name** | hexadecan-1-ol |
| **EC No.** | 253-149-0 |
| **TSCA Name** | 1-Hexadecanol |
| **Molecular Formula** | C16H34O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Memo:** MERGED JAN 2006

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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |

| | |
|---|---|
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Hexadecanol
**Smiles Code:** OCCCCCCCCCCCCCCCC
**Mol. Formula:** C16 H34 O1
**Mol. Weight:** 242.45

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-hexadecanol, CAS 36653-82-4 are 100% linear.

The substance comprises >=95% C16. Components of even chain length, in the range C14-C18 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Hexadecanol (9CI) (CA INDEX NAME)
Cetaffine
Cetal
Cetalcos
Cetalol CA
Cetanol
Cetyl alcohol
Cetylic alcohol
Cetylol
CO 1695
CO 1695F
Conol 1695
Crodacol C
Crodacol CAS
Crodacol CAT
Elfacos C
Epal 16
Ethal

Ethol
Hexadecanol
Hexadecyl alcohol
Hyfatol 16
Hyfatol 16-85
Hyfatol 16-95
Kalcohl 60
Kalcohl 6098
Kalcol 68
Lanette 16
Lanol C
Laurex 16
Lipocol C
Lorol 24
Lorol C 16
Loxanol K
Loxanol K extra
Loxanwax SK
n-1-Hexadecanol
n-Cetyl alcohol
n-Hexadecanol
NAA 44
NSC 4194
Palmitic alcohol
Palmityl alcohol
Alcohol, C16
Hexadecan-1-ol
1-Cetanol
Adol 52
Adol 52NF
Adol 54
Alfol 16
Alfol 16RD
Atalco C

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-hexadecanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to 10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (8) (60) (91)

## 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

## 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

## 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

## 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 13 Construction materials and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 14 Corrosion inhibitors
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 15 Cosmetics
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 35 Lubricants and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 41 Pharmaceuticals
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 50 Surface-active agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (98)

## 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

## 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-hexadecanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-AUG-2005

## 2.1 Melting Point

**Value:** = 50 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The cited source of the value is a recognised source of physico-chemical data.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (99)

**Value:** ca. 46 - 52 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Method:** other
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** UNION DERIVAN S.A. VILADECANS
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. A source of higher reliability is available.
19-SEP-2005

**Value:** = 49 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
19-SEP-2005 (64)

**Value:** = 49.3 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
19-SEP-2005 (44)

## 2.2 Boiling Point

**Value:** = 334 - 344 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (54)

**Value:** = 300 - 320 degree C

**Method:** other
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** UNION DERIVAN S.A. VILADECANS
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. A source of higher reliability is available.
04-JAN-2005

**Value:** = 344 degree C at 1013 hPa

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (99)

## 2.3 Density

**Type:** density
**Value:** = .8176 g/cm³ at 50 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (44)

**Value:** = .818

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
21-OCT-2005 (92)

**Type:** density
**Value:** ca. .81 g/cm³ at 60 degree C

**Method:** other
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** UNION DERIVAN S.A. VILADECANS
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
04-JAN-2005

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000014 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (18)

**Value:** = 1.3 hPa at 123 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
04-JAN-2005 (95)

**Value:** = .00000407 hPa at 30 degree C

**Method:** other (measured)
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
04-JAN-2005 (55) (85)

**Value:** = 1.33 hPa at 122.7 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (2) valid with restrictions
This information was obtained from the public IUCLID 2000 CD-ROM. The cited reference is a recognised source of physico-chemical data.
04-JAN-2005 (53)

**Value:** = .000016 at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
09-AUG-2005 (3)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 6.65

**Method:** other (measured): Reverse-phase HPLC with mass spectrometry
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures. Test conditions Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm Mobile Phase: Solution A: methanol:ethanol:water 70:15:15 Solution B: methanol:ethanol:water 95:5:0. 100% A for 1 min. Gradient to 100% B at 6.67% per min. 100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).
**Reliability:** (2) valid with restrictions
Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (14)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .013 mg/l at 25 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for water solubility values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (85) (104)

**Solubility in:** Water
**Value:** = .03 mg/l

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
04-JAN-2005 (54)

**Value:** = .12 mg/l at 25 degree C

**Method:** other: berechnet
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (97)

**Value:** = .0134 mg/l at 25 degree C

**Method:** other: berechnet
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (47)

**Value:** = .0143 mg/l at 25 degree C

**Method:** other: berechnet
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The water solubility is estimated to be 0.043 mg/l at a loading rate of 1000 mg/l.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
11-SEP-2005 (1)

**Value:** = .024 mg/l at 25 degree C

**Method:** other: gemessen (keine weiteren Angaben)
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (103)

**Value:** = .008 mg/l at 34 degree C

**Method:** other: gemessen ueber radioaktive Markierung
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
05-JAN-2005 (52)

**Value:** = .0155 mg/l at 43 degree C

**Method:** other: gaschromatographisch gemessen
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
04-JAN-2005 (47)

**Solubility in:** Water
**Value:** = .043 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.043 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
17-OCT-2005 (3)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 135 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** while not stated, it is considered likely that this is a value obtained in a closed cup test by comparison with other measured data.
**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
04-JAN-2005 (48)

**Value:** ca. 175 degree C
**Type:** open cup

**Method:** other
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** UNION DERIVAN S.A. VILADECANS
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
04-JAN-2005

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Type:** other: UV lamp

**Method:** other (measured): microphotoreactor developed by Lotz et al, modified by Kotzias et al.
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Exposure period: 17 hours
Temperature: 15 degrees C
Test concentration: 1680 ng/g Silica gel
UV lamp at 290 nm
**Result:** 3.1% mineralisation (CO2), and ~0.5% (organic fragments)
**Reliability:** (4) not assignable
Documentation insufficient for assessment. A source of higher reliability is available.
09-JAN-2005 (26)

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 23.84660E-12 cm3/molecule.sec
Half-life: 16.2 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
21-DEC-2005 (5)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in respect of hydrolysis. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
09-JAN-2005

### 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

**Method:** The EU samples were obtained during 2001-2 from municipal waste water treatment plants. Each was obtained over a 24-hour period, and preserved by addition of formalin at the time of sampling.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivatisation Liquid-chromatography-mass spectrometric (LCMS) technique.

Samples from Canada were grab samples obtained during August 2003, and were preserved with formalin.

**Remark:** The study is of effluent monitoring of 20 biofilm and activated sludge wastewater treatment plants from Europe (12) and Canada (8) receiving predominantly municipal effluent. Concentrations of alcohols and alcohol ethoxylates were measured.

**Result:** In the results, Provinces are indicated as 2-letter abbreviations. Results are presented as µg/L concentrations as:

| Location: Treatment Type | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Vernon, BC: TF | 0.393 | 0.174 | 0.428 | 0.886 | 0.452 | 0.718 | 3.051 |
| Kelowna, BC: AS | 0.243 | 0.102 | 0.107 | 0.181 | 0.095 | 0.121 | 0.849 |
| Toronto, ON: AS | 0.027 | 0.235 | 0.548 | 0.312 | 0.883 | 0.492 | 2.497 |
| La Prairie, QC: AS | 0.070 | 0.030 | 0.029 | 0.041 | 0.057 | 0.068 | 0.295 |
| Victoriaville, QC: AS | 0.069 | 0.019 | 0.014 | 0.048 | 0.026 | 0.109 | 0.285 |
| Paris, ON, AS | 0.036 | 0.030 | 0.033 | 0.059 | 0.083 | 0.060 | 0.301 |
| Cardston, AB: RBC | 1.251 | 0.961 | 3.354 | 3.257 | 3.180 | 2.174 | 14.2 |
| Waterloo, ON: AS | 0.301 | 0.122 | 0.156 | 0.172 | 0.160 | 0.127 | 1.038 |

TF = trickling filter
AS = activated sludge
RBC = rotating biological contactor

Data from activated sludge plants in Europe:

Total alcohol µg/L

| Location | C12 | C13 | C14 | C15 | C16 | C18 | Total |
|---|---|---|---|---|---|---|---|
| Northwich, UK | 0.468 | 0.319 | 0.305 | 0.154 | 0.485 | 0.591 | 2.322 |
| Cannock, UK | 0.104 | 0.087 | 0.069 | 0.084 | 0.179 | 0.318 | 0.841 |
| Rushmoor, UK | 0.134 | 0.104 | 0.095 | 0.125 | 0.338 | 0.408 | 1.204 |
| Kralingse Veer, NL | 0.410 | 0.147 | 0.138 | 0.125 | 0.368 | 0.138 | 1.326 |
| De Meern, NL | 0.282 | 0.208 | 0.174 | 0.155 | 0.472 | 0.239 | 1.53 |
| Horstermeer, NL | 0.360 | 0.211 | 0.212 | 0.136 | 0.598 | 1.209 | 2.726 |
| Estepona, ES | 0.214 | 0.073 | 0.182 | 0.148 | 0.999 | 1.144 | 2.76 |
| La Vibora, ES | 1.179 | 0.533 | 1.741 | 1.181 | 4.172 | 2.426 | 11.23 |
| Munich, DE | 0.010 | 0.023 | 0.007 | 0.034 | 0.005 | 0.008 | 0.087 |
| Torino, IT | 0.070 | 0.094 | 0.057 | 0.058 | 0.419 | 0.038 | 0.736 |
| Robecco, IT | 0.092 | 0.130 | 0.072 | 0.206 | 0.187 | 0.266 | 0.953 |

Ratingen, DE 0.046 0.052 0.033 0.083 0.037 0.068 0.319
(usual country and US state designators)
Results for all carbon numbers are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP monitoring studies conducted to a high standard.

21-DEC-2005 (15)

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 242.4
Data temperature 25 deg C
Log Kow 6.65
Water Solubility 0.013 mg/l
Vapour pressure 0.0014 Pa
Melting point 50 deg C
half life in air 16.2 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 0.13% |
| Soil | 97.6% |
| Water | 0.03% |
| Fish | 5.51E-03% |
| Sediment | 2.17% |

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 9.88 | 0.00125 | 1.34E-05 |
| % in water | 1.25 | 2.98 | 0.0103 |
| % in sediment | 40.7 | 97 | 0.335 |
| % in soil | 48.2 | 0.00609 | 99.7 |

The results reflect that the ultimate fate of 1-hexadecanol is dependent on its route of release into the environment. 1-Hexadecanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-hexadecanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and

principles.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

## 3.3.2 Distribution

**Method:** Measurement of the sorption of five alcohols onto a mixture of activated sludge and river water suspended solids.
River water was collected from River Gowy, Ellesmere Port, on two successive days and mixed then sterilised. It contained 12 mg/L suspended solids.

Activated sludge was obtained from a municipal waste water treatment plant. The mixed liquor suspended solids content was determined to be 2940 mg/L. Total organic carbon was 880 mg/L. The mixture was sterilised, allowed to settle, and a simulated effluent was prepared to give 30 mg/L suspended solids. The fraction of organic carbon was 0.167. The vessel was spiked with TS to give ca. 100 µg/L. The test system was stirred for 24 h, which was sufficient to give equilibrium.

The mixed settled activated sludge with river water with up to 72 h equilibration.
**Remark:** The results for five substances are considered alongside each other since the results of the whole study are useful for comparison purposes.
The data for the alcohol ethoxylates obtained in the study do not need to be included in this summary.
**Result:** Alcohol sorption coefficients showed some time dependence, reaching a plateau by 72 h. C15 was found to be an unexplained outlier. The 72 h results were:

| C | 12 | 14 | 15 | 16 | 18 |
|---|---|---|---|---|---|
| Kd | 3000± 80 | 8490± 920 | 3080± 270 | 23800 ±3200 | 78700 ±5400 |
| Koc | 17980 | 50830 | - | 143000 | 471000 |
| log Koc | 4.25 | 4.71 | | 5.15 | 5.67 |

These data (neglecting the C15) can be interpreted as a QSAR in the usual way as:

Log Koc = 0.11 + 0.77 log Kow

R2 = 0.994

The result is in line with typical QSARs of this type.
**Test substance:** Linear alcohols labelled with 14-C, radiochemical purity 99%
**Reliability:** (2) valid with restrictions
Although not a SIDS end point, this study is considered to be the best study of Koc for these carbon numbers.
21-DEC-2005 (69)

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 6.65was used in the TGD calculation methods.

**Result:** TGD Hydrophobics method: Koc = 307000
TGD Non-hydrophobics method: Koc = 30100
TGD Alcohols method: Koc = 1240
SRC PCKOCWIN method: Koc = 3790

**Test substance:** As prescribed by section 1.1-1.4

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods

28-DEC-2005 (5)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 17.1 mg/l related to Test substance
**Contact time:** 29 day(s)
**Degradation:** = 62 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 6 day(s) = 10 %
16 day(s) = 52 %
28 day(s) = 62 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were fulfilled: (1) degradation rate of the reference substance had reached a level of 60% within 14 days, (2) parallel assays did not differ by more than 20%, (3) CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test, (4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.

**Result:** Kinetic of control substance: 6 days = 40%
16 days = 102%
28 days = 105%
The test substance attained 62% degradation over the test period. However, the 60% pass level was not reached within the 10 day window, therefore it cannot be considered

readily biodegradable.
**Test condition:** Concentration of activated sludge: 30 mg dry matter/l
Test volume: 3 l
Temperature: 21°C
pH: not reported
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (59)

**Type:** aerobic
**Inoculum:** other: activated sludge, predominantly domestic
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 76 % after 28 day(s)
**Result:** inherently biodegradable
**Kinetic:** 7 day(s) = 40 %
14 day(s) = 59 %
21 day(s) = 67 %
28 day(s) = 76 %
**Control Subst.:** other: Sodium acetate

**Method:** other: ISO 10708 (BODIS) and RDA Blok Test
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test method used is based on OECD test method 301D and the RDA-Blok-Test. Mineral medium was inoculated with activated sludge and stabilized for one week at 20-25 C with continuous stirring. After stabilisation, 200 ml of test medium was filled into 300 ml bottles, aerated until O2 saturation was reached and spiked with test substance by directly weighing into the test vessels. Vessels were filled 2/3, stoppered and shaken continuously at 20-25 C.
Degradation was followed by weekly measurements of BOD using an O2-electrode. Oxygen consumption resulting from biodegradation of the test substance was corrected by oxygen uptake of blank inoculum. Degradation rate was calculated as % BOD/COD.
**Remark:** The validity criteria were fulfilled: (1) degradation rate of the reference substance had reached a level of 60% within 14 days, (2) total oxygen uptake in blanks after the first week was lower than 3 mg O2 and lower then 1 mg O2 in the following weeks, (3) residual concentration of O2 in test bottles did not fall below 0.5 mg/l.
However, the parallel assays did not fall within the acceptable 20% range. On day 28, the % degradation for the three replicates was 71%, 91% and 67%.
**Result:** Kinetic of control substance:
7 days = 81%
14 days = 95%
21 days = 97%
28 days = 98%
The test substance attained 76% degradation over the test period. However, the 60% pass level was not reached within the 10 day window, therefore it cannot be considered readily biodegradable. However, significant degradation was observed therefore the substance is considered to be inherently biodegradable.
**Test condition:** Concentration of activated sludge: 30 mg dry matter/l

Test volume: 200ml
Temperature: 20-25 C
pH: not reported

**Reliability:** (2) valid with restrictions
The test failed to meet one of the validity criteria of the test guideline.

17-OCT-2005 (42)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 61 % after 31 day(s)
**Result:** inherently biodegradable
**Kinetic:**
4 day(s) = 27 %
10 day(s) = 47 %
17 day(s) = 59 %
24 day(s) = 60 %
31 day(s) = 61 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** There is no information given on the validity criteria.
**Result:** Kinetic of control substance:
4 days = 47.1%
10 days = 58.1%
17 days = 60.5%
24 days = 61.2%
31 days = 62.2%
The test substance attained <60% degradation over the test period therefore it cannot be considered readily biodegradable.
**Reliability:** (4) not assignable
The information reported is insufficient to assess the validity of this study.

17-OCT-2005 (96)

**Type:** anaerobic
**Inoculum:** other: activated sludge from municipal sewage digester
**Concentration:** 10 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 97 % after 28 day(s)

**Method:** other
**Year:** 1985
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Model sludge digester utilizing 14C-radiolabelled test compound and conducted at mesophilic temperatures (35 C)
**Remark:** The publication describes in detail the test system and method used to evaluate the anaerobic biodegradability of several materials including 14C-cetyl alcohol obtained from Amersham-Buchler in Germany.
**Result:** Total gas production for the fatty alcohol was 97.1% (25.1% as 14CH4 and 72% as 14CO2). Approximately 4% of the starting material remained in the sludge and approximately 0.5% was in the supernatant.
**Test condition:** Concentration of inoculum: 45 g of centrifuged activated sludge (corresponding to 3 g of dry sludge)
Test volume: 300 ml
Temperature: 35 C
pH: Adjusted to 7 at start of test
**Reliability:** (2) valid with restrictions
Well-documented scientific study.
30-AUG-2005 (84)

**Type:** anaerobic
**Inoculum:** other: municipal sewage digester sludge fortified with activated sludge
**Concentration:** 1 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 90.1 % after 28 day(s)

**Method:** other
**Year:** 1996
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Batch test system using C14-labelled material modified after Steber and Wierich 1987
**Remark:** The method involves a batch test system with a domestic wastewater treatment sludge inoculum. The evolution of radiolabeled carbon dioxide and methane are monitored. The test temperature is 35 degrees C. Starting solids levels of the test sludge ranged between 24 and 29 g/L.
C14-hexadecanol (labeled in the first carbon) was obtained from Sigma Chemical in St. Louis, MO (purity >98%) and hexadecanol was obtained from American Tokyo Kasei Inc. in Portland, OR. The final ratio of C14 -CO2 to C14 -CH4 in the gas produced was 3.3 to 1. The mechanism of hexadecanol biodegradation would be catabolized by beta oxidation to form acetate. Hexadecanol degradation exhibited first-order kinetics.
**Result:** Total gas production for hexadecanol was 90.1% (69.1% as 14CO2 and 21.0% as 14CH4). Approximately 9% of the starting material remained with the solids and 0.5% remained in solution.
**Reliability:** (2) valid with restrictions
Well-documented scientific study.
30-AUG-2005 (65)

**Type:** aerobic
**Inoculum:** predominantly domestic sewage
**Concentration:** .05 mg/l related to Test substance
**Degradation:** = after 5 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroessen: Konzentration der Testsubstanz, CO2-Entwicklung radioaktiv markierte Testsubstanz.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** 25 Grad C; Ansatz geruehrt
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (26)

**Type:** aerobic
**Inoculum:** predominantly domestic sewage
**Concentration:** 50 µg/l related to Test substance
**Degradation:** = 28 % after 5 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroesse: 14CO2-Entwicklung
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** U-14C Hexadecanol; Ruehren; T = 24-26 Grad C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (24)

**Type:** aerobic
**Inoculum:** predominantly domestic sewage
**Concentration:** 50 µg/l related to Test substance
**Degradation:** = 37 % after 5 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroesse: 14CO2-Entwicklung
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** U-14C Hexadecanol; Ruehren; T = 24-26 Grad C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (25)

**Type:** aerobic
**Inoculum:** other bacteria: Marines Sediment (adaptiert)
**Concentration:** 1.7 mmol/l related to Test substance
**Degradation:** = 96 % after 42 day(s)
**Kinetic:** 25 day(s) = 62 %

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroesse: substanzspezifische Analytik (IR-Spektroskopie)

Werte aus graphischer Darstellung entnommen
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 16 Grad C; Schuetteln
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (46)

**Type:** anaerobic
**Inoculum:** other bacteria: Marines Sediment (adaptiert)
**Concentration:** 1.7 mmol/l related to Test substance
**Degradation:** = 90 % after 121 day(s)
**Kinetic:** 63 day(s) = 67 %

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroesse: substanzspezifische Analytik (IR-Spektroskopie)
Werte aus graphischer Darstellung entnommen
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 16 Grad C; Schuetteln
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (46)

**Type:** anaerobic
**Inoculum:** other bacteria: Mischung aus Belebtschlamm und Faulschlamm
**Concentration:** 10 mg/l related to Test substance
**Degradation:** = 97.1 % after 28 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Messgroesse: Gasentwicklung (14CO2 & 14CH4)
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** 35 Grad C; radioaktiv markierte Testsubstanz; periodisches Umruehren des Testansatzes (alle 12 h)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (83)

**Degradation:** = 0 % after 5 day(s)

**Method:** other: BSB-Bestimmung nach AFNOR-Richtlinie NF T90/103 (1969)
**Year:** 1969
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Abbaugrad: 0 % (Sauerstoffmangel durch Bildung eines Oberflaechenfilms?)

Einsatzkonzentration: nicht angegeben
Inokulum: nicht angegeben
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (20)

**Inoculum:** activated sludge, non-adapted
**Concentration:** 500 mg/l related to Test substance
**Degradation:** = 0 % after 1 day(s)

**Method:** other: Warburg-Respirometer
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Abbauversuche mit drei Belebtschlaemmen unterschiedlicher Herkunft
der Stoff wirkte auf jeden der getesteten Belebtschlaemme toxisch (Sauerstoffmangel durch Bildung eines Oberflaechenfilms?)
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** 20 Grad C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (29)

**Inoculum:** predominantly domestic sewage
**Concentration:** 73 mg/l related to Test substance
**Degradation:** = 14.3 % after 20 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** durchgehender Oberflaechenfilm (begrenzte Bioverfuegbarkeit)
Messparameter: Gewichtsverlust des eingesetzten Hexadecanols nach Methanolextraktion
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 20 Grad C; schwache Belueftung
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (56)

**Inoculum:** predominantly domestic sewage, adapted
**Concentration:** 76 mg/l related to Test substance
**Degradation:** = 8.6 % after 37 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** durchgehender Oberflaechenfilm (begrenzte Bioverfuegbarkeit)

Messparameter: Gewichtsverlust des eingesetzten Hexadecanols nach Methanolextraktion
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 20 Grad C; schwache Belueftung
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (56)

**Inoculum:** other bacteria: Pseudomonas sp. (adaptiert)
**Concentration:** 800 µmol/l related to Test substance
**Degradation:** ca. 66 % after 2 day(s)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Alkohole (C10 - C18) als Gemisch geprueft; Einzel-Abbauraten aus GC-Peaks bestimmt; Abbau-Werte aus Graphik ermittelt
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** Inkubation in Minimalmedium mit Gemisch aus Alkoholen (C10, C12, C14, C16 & C18) in Konzentrationen zu je 0.8 mmol/l; geschuettelt; T = 30 Grad C
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (102)

**Method:** Laboratory continuous activated sludge study.

4 mg/L of TS
20°C
Hydraulic residence time (HRT) 6 h
Sludge retention time (SRT) 10 d

The feed to the sludge unit was of sterile synthetic sewage and AE concentrate and non-sterile tap water.

19 d acclimation was used, followed by 10 days of evaluation. At the start the unit was seeded with sewage treatment plant (STP) activated sludge.

The unit was sampled several times per week, and the samples were analysed immediately.

Analytical recovery of the alcohols was high.

The results showed that the CAS unit was running in a similar way to a full scale STP.
**Remark:** This paper describes mainly the properties of alcohol ethoxylates (AE) but contains valuable data about the properties and environmental exposures of alcohols themselves. This study should not be considered as a study of alcohols alone, but is important in that it indicates that the extent

of removal of alcohols from an exposure route that can be anticipated. This extent is high. The waste water organisms were exposed principally to ethoxylates, but the alcohols would be generated by the degradation of the ethoxylates.

**Result:** Results are corrected for control values.

| Alcohol | Conc. in effluent ng/L | Conc. in sludge µg/g | %removal |
|---|---|---|---|
| C12 | 18 | 0.6 | 98.6 |
| C13 | 21 | 0.7 | 99.5 |
| C14 | 5.5 | 0 | 99.6 |
| C15 | 2.9 | 1.1 | 99.8 |
| C16 | 1.6 | 0.01 | 99.5 |
| C18 | 58 | 0.7 | 99.1 |
| Total | 130 | 2 | 99.4 |

| | |
|---|---|
| Total elimination of ethoxylates | 97.4 |
| Total in waste sludge solids | 2.0 |
| Total in suspended solids | 0 |

This shows that most of that which does not degrade (itself a small amount) is in the solids.

**Test substance:** 2:1 mixture of NEODOL 25-7 and GENAPOL T110

Alkyl chain distribution

| C | Mol ratio |
|---|---|
| 12 | 1 |
| 13 | 2 |
| 14 | 2.3 |
| 15 | 1.8 |
| 16 | 1.1 |
| 18 | 2.9 |

**Reliability:** (2) valid with restrictions
OECD 303. Public domain paper based on a fuller Shell laboratory report.

21-DEC-2005 (86)

**Method:** The study was a batch-mode activated sludge die-away system. Two treatments consisting of 1 litre each of biologically active sludge were prepared for each test substance. The 14-C alcohols were dissolved in methanol, which was diluted in water and dosed into the sludge in 2-litre flasks.

Disappearance of parent, formation and disappearance of metabolites, uptake into biomass and mineralization to 14-C CO2 were monitored over time.

Activated sludge from a municipal WWTP was obtained, and used at 2500 mg/L.

The TS was dosed at 0.05 µM: this is equivalent to 9.3µg/L (C12), 10.0 µg/L (C14), 10.7 µg/L (C16); added to flasks at 20°C.

**Remark:** The results for three substances are considered alongside each other since the results of the whole study are useful to show the consistency of the results.

**Result:** Recoveries were high.

After 48h incubation:

| C | Parent | metabolites | Water | Solids | CO2 |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| C12 | 0.8 | 5.9 | 3.5 | 20.7 | 73.9 |
| C14 | 1.3 | 6.3 | 2.0 | 21.0 | 76.7 |
| C16 | 2.6 | 11.5 | 2.1 | 17.0 | 65.3 |

Concentrations were modelled with the equation
C = Ae^(-k1t) + B(e^-k2t)
(a two compartment first order decay model)

| % | A | k1 h-1 | B | k2 h-1 |
|---|---|---|---|---|
| C12 | 82±2 | 113±8 | 9±1 | 0.36±0.1 |
| C14 | 82±2 | 87±5 | 12±1 | 0.30±0.1 |
| C16 | 41±3 | 103±23 | 48±2 | 0.43±0.04 |

The results show the high biodegradability of C12 to 16 alcohols in activated sludge.

**Test substance:** Radiolabelled (14C) C12, C14 and C16 alcohols.

**Reliability:** (2) valid with restrictions
Non-standard study conducted to a scientifically sound method.

21-DEC-2005 (87)

**Method:** Effluent monitoring of waste water treatment plants receiving predominantly municipal effluent. Concentration of alcohols and alcohol ethoxylates were measured.

Twenty-four hour composite samples of influent and effluent were collected from each of the locations from three days. They were preserved with formalin at the time of collection. These were composited in proportion to flow.

Samples of 4 litres ware obtained and extracted onto a succession of cartridges, followed by solvent elution. Quantitative analysis of the eluates was by a derivitisation Liquid-chromatography-mass spectrometric (LCMS) technique.

**Result:** Influent (In), effluent (Eff) values in ug/l, and % removal of alcohols are indicated in the table below, with alcohol data considered in two groups. The State in which the WWTP is found is indicated by the usual 2-letter abbreviation.

| | | C12-15 OH In | eff | % | C16-18 OH in | eff | % |
|---|---|---|---|---|---|---|---|
| TX | Lagoon | 297 | 2 | 99.3 | 92.7 | 2.4 | 97.4 |
| NJ | Oxidation Ditch | 249 | 0.7 | 99.7 | 181 | 0.8 | 99.6 |
| OH | Rotating biological contactor | 157 | 0.1 | 0.06 | 77 | 0.07 | 99.9 |
| IA | Trickling filter | 499 | 2.0 | 99.6 | 354 | 2.3 | 99.4 |
| MO | Trickling filter | 532 | 4.9 | 99.1 | 315 | 9 | 97.3 |
| KS | Lagoon | 67.5 | 1.1 | 98.4 | 35.4 | 2.2 | 93.8 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| CA | Activated sludge | 20.05 | 0.2 | 99.9 | 169 | 0.4 | 99.8 |
| OR | Activated sludge | 92.9 | 0.2 | 99.8 | 133 | 0.6 | 99.5 |
| AZ | Oxidation ditch | 702 | 0.3 | 100 | 394 | 0.5 | 99.9 |

Results for the carbon number groups are considered alongside each other to enable the context of every data point to be seen. In the overall interpretation of the data, the results have been used with those from other studies to determine the contribution of measured alcohol concentrations from various sources.

**Reliability:** (2) valid with restrictions
Non-GLP studies conducted to a high standard.

21-DEC-2005 (72)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 3 day(s)
**Concentration:** 48 µg/l
**BCF:** = 56
**Elimination:** yes

**Method:** other
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Five fish, 5-6 cm long, about 1.5 g in weight were exposed in 10 litres of water at 20-25 degC.
**Remark:** Bioaccumulation potential of hexadecanol was assessed in a static renewal, closed system, using radiolabeled test material. The concentration of test substance was 50 ug/l, which is approximately four times the water solubility. The 14C measurement in the fish and the test water does not distinguish between parent compound and its transformation products, and so the accumulation factor is a measure of all the radioactive compounds present in the system. No attempt was made to determine kinetic information or whether steady state was achieved.
As a result, the measured BCF value of 56 may be called into question. Testing above the limit of solubility increases the chances of under-estimating the BCF value whilst detecting for total 14C increases the chances of over-estimating the BCF value. Measured value for hexadecanol can not be relied upon as being definitive.
**Reliability:** (3) invalid
Not valid due to use of total radioactivity, testing above water solubility, no attempt to determine steady state conditions

09-JAN-2005 (27)

**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**BCF:** = 507 - 1550
**Year:** 1995
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The accumulation of Hexadecanol by B. rerio was examined. Tests were performed with Hexadecanol/DMSO, Hexadecanol/DMSO/Tween 85, Hexadecanol/Tween 85 and Hexadecanol/Tween 80 but results are only reported for Hexadecanol/DMSO since mortality of control and test animals was unacceptable in the other tests.
Hexadecanol was weighed out and dissolved in dimethyl sulphoxide to produce 1, 3, 10, 30 and 100 mg/l solutions. Radiolabelled Hexadecanol (12.5 mCi/mmol, 9-14C) was dissolved in acetone. Labelled Hexadecanol was added to glass vials and the acetone evaporated. 'Cold' Hexadecanol was then added. Five litres of test solution were prepared for each test concentration.
500 ul of each stock solution was sonicated into 500 ml of carbon-filtered Wirral tap water (test medium). This was diluted to 5 litres with more carbon-filtered Wirral tap water to produce the final concentrations. Ten fish were exposed at each of the 5 concentrations. Test solutions were renewed daily.

**Remark:** Measurements of hexadecanol concentrations in fish were by 14C. Specific analysis of intact hexadecanol were not undertaken. Reported concentrations of hexadecanol in fish assumed all the radiolabelled material was intact unless stated otherwise.

**Result:** Estimates of soluble Hexadecanol concentrations were made by centrifugation of aqueous samples (40000 g for 30 minutes) and by filtration (2 * through a 0.22 um membrane filter). These estimates of soluble concentrations were used to calculate BCF values. However even these "dissolved" concentrations were greater than water solubility, especially at higher loading rates.

| | |
|---|---|
| Filtered 0.03 mg/l | BCF = 1033 +/- 333 |
| Centrifuged 0.02 mg/l | BCF = 1550 +/- 500 |
| Filtered 0.08 mg/l | BCF = 563 +/- 50 |
| Centrifuged 0.06 mg/l | BCF = 750 +/- 67 |
| Filtered 0.15 mg/l | BCF = 833 +/- 287 |
| Centrifuged 0.16 mg/l | BCF = 781 +/- 269 |
| Filtered 0.39 mg/l | BCF = 736 +/- 369 |
| Centrifuged 0.33 mg/l | BCF = 870 +/- 436 |
| Filtered 1.16 mg/l | BCF = 507 +/- 209 |
| Centrifuged 0.67 mg/l | BCF = 878 +/- 361 |

BCF's based on estimated soluble concentrations are reasonably similar all falling in the range 500-1000.

**Test condition:** Test temperature = 18.5-20.5 C
pH = 7.1-7.7
Dissolved Oxygen (mg/l) = 6.5-7.8
Total Hardness (as CaCO3 mg/l) = 84-95

**Reliability:** (3) invalid
Not valid due to use of total radioactivity, estimation of exposure concentrations, no attempt to determine if steady state conditions were achieved.

09-JAN-2005 (90)

**Species:** other: activated sludge

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Bioakkumulationsfaktor:
Belebtschlamm: 1300 (5 d; T = 24-26 Grad C; Ruehren; aerob experimentell bestimmt mit 50 ug/l U-14C Hexadecanol, keine substanzspezifische Analytik, nur Radioaktivitaet gemessen (14C-Einbau in Biomasse?).
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (25)

**Species:** other: see remarks

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Bioakkumulationsfaktoren:
Chlorella fusca (Alge): 17 000 (24 h; T=20-25 Grad C; Schuetteln)
Belebtschlamm: 3170 (5 d; T = 24-26 Grad C; Ruehren; aerob)
Leuciscus idus melanotus (Goldorfe): 56 (3 d; T = 20-25 Grad C; Ruehren;
keine Fuetterung).
50 ug/l U-14C Hexadecanol; keine substanzspezifische Analytik, nur Radioaktivitaet gemessen (14C-Einbau in Biomasse?).
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
09-JAN-2005 (24) (26) (32)

**BCF:** = 45300

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 6.65 was used in the calculation
**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

21-DEC-2005 (5)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** semistatic
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** >= .4
**LC50:** > .4
**Limit Test:** yes

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The solubility of C16 alcohol (hexadecanol) is about 0.01 mg/l, therefore the LC50 was not achieved at the solubility limit.
**Result:** RESULTS: EXPOSED
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Wetton 1996c.
**Test condition:** TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Donnington Fish Farm, Upper Swell, Gloucestershire, UK
Weight: 1.20 g
Feeding: Commercial trout pellets
Pretreatment: Acclimatised to test conditions for 1 week prior to test
Feeding during test: None
Control group: 1 control and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTION
not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels aerated via narrow bore glass tubes
Alkalinity: 80 mg/l
Hardness: 136 mg/l CaCO3
Conductance: 405 uS/cm
TEST SYSTEM
Concentrations: 0.4 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 13-14 C
Dissolved oxygen: 9.2 - 10.1 mg O2/l
pH mean: 7.4 - 7.9
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 16 hours light and 8 hours darkness
TEST PARAMETER: Mortality

SAMPLING: Mortalities and adverse reactions to exposure were recorded at 3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (100)

**Type:** semistatic
**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** > 10
**Limit Test:** no

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1995
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Five acute toxicity tests were conducted with hexadecanol using four different preparation methods. None of the tests resulted in significant mortality due to the action of hexadecanol. Although the deaths in the control (typicaly 10-30%) complicate the interpretation, the data demonstrate that the 96 hour LC50 was greater than the highest concentration tested (10 mg/L). This is about 1000 times the water solubility of hexadecanol.
**Source:** Unilever, 1995.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility available
21-JUL-2005 (90)

**Type:** static
**Species:** Oncorhynchus kisutch (Fish, fresh water, marine)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** > 10

**Remark:** keine toxische Wirkung bei 10 mg/l
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 11 Grad C; pH 7.2
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (57)

**Type:** static
**Species:** Oncorhynchus tschawytscha (Fish, fresh water, marine)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** > 10

**Remark:** keine toxische Wirkung bei einer Konzentration von 10 mg/l
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 11 Grad C; pH 7.2

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (57)

**Type:** static
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 5
**Unit:** mg/l **Analytical monitoring:**
**LC0:** = 500

**Method:** other: keine naeheren Angaben
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** der Stoff wurde von den Fischen aufgenommen und offenbar unveraendert ausgeschieden, die durch Filmbildung reduzierte Sauerstoffzufuhr verursachte bei den Tieren Stresserscheinungen keine toxische Wirkung bis 500 mg/l.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test substance:** Emulsion von 1-Hexadecanol in Wasser
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
17-OCT-2005 (11)

**Type:** static
**Species:** Ptychocheilus oregonensis (Fish, fresh water)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** > 10

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** keine toxische Wirkung bei einer Konzentration von 10 mg/l
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
20-OCT-2005 (57)

**Type:** static
**Species:** Salmo irideus (Fish, fresh water)

**Remark:** Hexadecanol has no significant effect on either respiration or total resting metabolism of Salmo irideus. When the fish were confined, oxygen consumption was increased only during the recuperation period in pure water and 2 hr following exposure to 10, 100, and 1000 ppm hexadecanol. Under semiconfinment conditions, 2-3 ppm hexadecanol had no effect on total resting metabolism.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the

CAS number.
17-OCT-2005 (35)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (4)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EbL50 :** = 676
**ErL50 :** > 980
**Limit Test:** no

**Method:** other: DIN 38412 part 9.
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of water constituents on green algae (Algae growth - inhibition-test)(L9); DIN 38412 part 9
This method corresponds to the OECD Guideline 201.
**Remark:** The water solubility of hexadecanol is about 0.01 mg/l, therefore the no effect level appears to be above the saturation limit. The loading rates were all markedly above the solubility, which suggests that the dose-response is artefactual.
**Result:** RESULTS: EXPOSED
Nominal/measured concentrations: nominal
Effect data/Element values:
ErL0 = 98 mg/l, ErL10 = 206 mg/l, ErL50 = >980 mg/l
EbL0 = 9.8 mg/l, EbL10 = 24 mg/l, ELC50 = 676 mg/l
Cell density data: cell densities increased from 3.7-4.3*10exp4 cells/ml after 24 hours to the following densities after 96 hours: 2.2*10exp6 (10 mg/l), 1.1*10exp6 (30 mg/l), 1.2*10exp6 (100 mg/l), 9*10exp5 (300 mg/l) and 9*10exp5 (1000 mg/l).
RESULTS CONTROL: cell density increased from 2.7*10exp4 after 24 hours to 2.1*10exp6 cells/ml after 96 hours.
**Source:** Guhl 1992c.
**Test condition:** TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen
Laboratory culture: not reported
Method of cultivation: not reported
Pretreatment: not reported
Controls: without test substance
Initial cell concentration: 1*10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: None
Other procedures: test substance directly weighed into test vessels
STABILITY OF TEST CHEMICAL SOLUTIONS: not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Test type: static test
Concentrations: 0, 10, 30, 100, 300 and 1000 mg/l
Renewal of test solution: none

Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 22 - 23 C
pH mean: not reported
Intensity of irradiation: 2000 lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
20-OCT-2005 (36)

**Species:** Scenedesmus subspicatus (Algae)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 10
**EC50:** = 690

**Method:** other: DIN 38412, Teil 9 (Algal growth inhibition test)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
**Test substance:** Active Matter = 98 %.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
11-SEP-2005

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria:Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** > 100

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
The MIC concentration appears to be above the SPARC estimated water solubility of Hexadecanol.
**Source:** Hattori 1987.
**Reliability:** (3) invalid
11-SEP-2005 (37)

**Species:** Aspergillus niger (Fungi)
**Exposure period:** 5 day(s)
**Unit:** mg/l **Analytical monitoring:**

**Method:** other: test for inhibition of spore germination
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For Chain length of alcohol C16: no antifungal activity up to 10 000 mg/l.
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l. Test duration: 5 d, 28 degr. C, pH 5.6
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
17-OCT-2005 (31)

**Species:** other bacteria: Bacteriophages
**Exposure period:** 30 minute(s)

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Chain length: C 16
Virentoxizitaet:
30 min. Inkubation mit Testsubstanz bei Raumtemperatur;
Parameter: Reduktion der plaque-forming units.
Bacteriophage phi 6: EC50 = >1 mM ( >242.4 mg/l)
Bacteriophage phi 23-1-a: EC50 = >1 mM ( >242.4 mg/l)
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
06-AUG-2005 (82)

**Species:** other bacteria: Clostridium botulinum
**Unit:** mg/l **Analytical monitoring:**
**MIC :** = 25

**Method:** other: statischer Zellvermehrungshemmtest nach Huhtanen, P.N., J. MilkFood Technol. 38, 762-763 (1975)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** MIC = minimale Hemmkonzentration
Testdauer: nicht angegeben
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** anaerobe Bedingungen
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000

CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (49)

**Species:** other bacteria: Mycoplasma gallisepticum
**Exposure period:** 144
**Unit:** mmol/l **Analytical monitoring:**

**Method:** other: statischer Zellvermehrungshemmtest
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** bei einer Konzentration von 0.064 mmol/l = 15.5 mg/l 97.9 % Wachstumshemmung
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 37 Grad C; Ethanol als Loesevermittler (<1 % v/v, nicht toxisch bei dieser Konzentration)
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (23)

**Species:** other bacteria: Mycoplasma pneumoniae
**Exposure period:** 144
**Unit:** mmol/l **Analytical monitoring:**

**Method:** other: statischer Zellvermehrungshemmtest
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** bei einer Konzentration von 0.064 mmol/l = 15.5 mg/l 90.8 % Wachstumshemmung
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 37 Grad C; Ethanol als Loesevermittler (<1 % v/v, nicht toxisch bei dieser Konzentration)
**Reliability:** (4) not assignable
4 Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
11-OCT-2005 (23)

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 24
**Unit:** mg/l **Analytical monitoring:**
**NOEC:** > 3

**Method:** other: statischer Zellvermehrungshemmtest
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** keine toxische Wirkung bei einer Konzentration von 12.4 uM (3 mg/l). Parameter: Truebungsmessung
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** T = 37 Grad C; Ethanol als Loesevermittler (keine Konzentrationsangabe, Kontrollen enthielten gleiche Menge Ethanol)
**Reliability:** (4) not assignable
4 Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are

based on the weight of evidence from various studies.
11-OCT-2005 (17)

**Species:** other fungi: see remarks

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** keine toxische Wirkung auf Aspergillus niger, Trichoderma viride, Myrothecium verrucaria, Candida albicans, Trichophyton mentagrophytes und Mucor mucedo bis zu einer Konzentration von 10 g/l.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Test condition:** Versuchzeitraum 30 h: Candida albicans, Mucor mucedo
5 d: A. niger, T. viride, M. verrucaria,
T. mentagrophytes
**Reliability:** (4) not assignable
Not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The overall conclusions concerning this end point are based on the weight of evidence from various studies.
29-DEC-2005 (30)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.
**Result:** No chronic effects would be expected for this substance.
**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (7)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of

hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (19)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** Cetyl alcohol was incompletely absorbed with 20% of the dose recovered unchanged from the faeces. Faecal excretion was complete within 48 hours. About 6% of the dose was in the form of glucuronic acid conjugate in the urine.

Absorption of palmitic acid was also incomplete with 30% receoverd unchanged from the faeces. There was no excretion of glucuronic acid metabolites.

**Source:** McIsaac & Williams, 1958
Hayes Consultancy Service Bromley, Kent

**Test condition:** In an investigation of the metabolism of cetyl alcohol and palmitic acid groups of 5 rats received doses of these materials in the diet. Urine and faeces were collected over a 5 day period. The total dose fed to the 5 rats was 2.5g each of cetyl alcohol or palmitic acid (ca 2g/kg).

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (58)

**Result:** Distribution results were reported for lauryl alcohol (98% pure). 95% of the dose adminstered was recovered from the application site at 24 hours after dosing. 0.13% remained in the body while 0.10% was excreted in the urine and faeces. 2.61% was excreted in expired air as CO2. The sum of these values indicates the amount of percutaneous absorption of lauryl alcohol(2.84%). The ratio of the amount of compound excreted via expired air to the amount absorbed is the expiratory excretion rate. It was 91% for lauryl alcohol. The respiratory excretion rates for all the other alcohols investigated were >65% although all the actual data is not reported.

Absorption decreased with increasing carbon chain length. The absorption rate was investigated in different solvents (squalene, castor oil, triethyl citrate (TEC). The percutaneous absorption rate of undiluted n-octanol was 50%, this was increased in squalene but decreased in castor oil or TEC. This was also reported with the other alcohols tested and the tendency was more pronounced at higher concentrations.

The degree of skin irritation was proportionally related to the degree of percutaneous absorption.

**Source:** Iwata et al, 1987
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 3 hairless mice were used. The 1-C14 labelled test substances were applied to the dorsal skin using a plaster for a 24 hour period. Immediately following application of the test material each animal was placed in a container to measure expiratory excretion. At the end of the exposure period the treated area of skin was excised and dissolved using tissue solubiliser. The carcass was homogenised in a blender wwith sodium hydroxide. An aliquot of the homogenate was then dried and combusted for determination of radioactivity.

The effect of different solvents and concentration of the solvent was also investigated. The role of skin irritation in absorption of test substance was also examined.

**Test substance:** n-octyl alcohol; n-decyl alcohol, lauryl alcohol and cetyl alcohol all radiolabelled (1-C14) and >98% pure.

**Conclusion:** Following skin application of lauryl alcohol about 2.84 % of the administered dose was absorbed. Of this absorbed dose >90% was excreted in expired air ($CO_2$). A similar trend was observed with the other alcohols tested. Absorption decreased with increasing carbon chain length and was affected by solvent and concentration.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (51)

**Remark:** hexadecanol is oxidised to hexadecanal which is rapidly oxidised to hexadecanoic acid. Hexadecanoic acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Test substance:** As prescribed hexadecanol

**Reliability:** (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including hexadecanol.

25-NOV-2004 (101)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: Sprague-Dawley CD
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: arachis oil
**Doses:** 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Hempstock 1996a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley)

- Source: Charles River, Margate, Kent, UK
- Age: 5-8 weeks
- Weight at study initiation: males 135-145g, females 127 -137g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg based on a range finding test.
- Doses per time period: single dose
- Volume administered or concentration: 10 ml/kg at a concentration of 200 mg/ml in arachis oil.
- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to gross pathological examination at the end of the observation period.

**Test substance:** Tradename Kalcol 6098

**Conclusion:** The rat oral LD50 for Kalcol 6098 is >2000 mg/kg. At this dose level there were no signs of toxicity.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (38)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: olive oil
**Doses:** 5000 g/kg
**Value:** > 5000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the observation period.

CLINICAL SIGNS: Slight sedation and piloerection were observed during the first 24 hours after dosing in all rats. The average body weight of the groups of male and female rats increased over the observation period.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Henkel KGaA 1981c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: rat (Wistar)
- Source: Winkelmann, Hanover, Germany
- Weight at study initiation: average body weight males 174g,

females 144g.
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 10 ml/kg as a 50% suspension in olive oil.
- Post dose observation period: 14 days.

EXAMINATIONS: Mortality and clinical signs were recorded. Body weights were taken before dosing and at 24 hours, 1 and 2 weeks after dosing. All rats were subject to gross necropsy at the end of the observation period.

**Test substance:** Tradename Lorol 16/Lanette 16

**Conclusion:** The rat oral LD50 for Lorol (Lanette) 16 is >5000 mg/kg. Clinical signs were confined to slight sedation and piloerection in the first 24 hours after dosing. Also reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (39) (50)

**Type:** LD50
**Species:** rat
**Strain:** other: Holzman albino
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: 20% w/v suspension in corn oil
**Doses:** 2.00, 3.99 and 7.96 g/kg
**Value:** > 7960 mg/kg bw

**Method:** other: Standard contract laboratory procedure.
**Year:** 1965
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no mortalities at any dosage level tested.

CLINICAL SIGNS: Diarrhoea was observed at all dose concentrations during the first 24 hours after dosing. All animals appeared normal within 48-hours post-dosage. Weight gain was within the normal limits.

NECROPSY FINDINGS: Gross necropsy revealed no remarkable signs.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.

**Source:** Scientific Associates, Inc. 1965e
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Holzman)
- Source: No reported
- Weight at study initiation: 204-254 g
- Group size: 5M+5F fasted
- Controls: No

ADMINISTRATION: gavage
- Doses: 2.00, 3.99 and 7.96 g/kg
- Doses per time period: single
- Volume administered or concentration: 20% suspension in cornoil
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality were recorded several times during the day of dosing and daily thereafter. All animals were necropsied and terminal body weights of survivors were recorded.

**Test substance:** Tradename Alfol 16
Tradename Alfol 16

**Conclusion:** The rat oral LD50 for Alfol 16 was >7.96 g/kg. The only clinical sign was diarrhoea at all dose levels in the first 24 hours after dosing. Gross necropsy revealed no remarkable changes. This study is reported in Iuclid 2000 erroneously giving the LD50 value as 7500 mg/kg.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

17-OCT-2004 (50) (76)

**Remark:** Summary report. Mouse oral LD50 3200 mg/kg, no further details available. Also reported in Iuclid 2000.

**Test substance:** No data

**Reliability:** (4) not assignable
Secondary reference.

18-OCT-2004 (50) (66)

**Remark:** Summary report of unpublished data provided by Fassett, originally reported in Patty's 2nd edition, 1963. Rat oral LD50 6.4-12.8 g/kg, mouse oral LD50 3.2-6.4 g/kg. No further details available.

**Test substance:** Cetyl alcohol, described in Patty, 1963 as a synthetic liquid C16 alcohol that may have contained impurities.

**Reliability:** (4) not assignable
Secondary reference.

06-AUG-2005 (66) (67) (68)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Summary report of unpublished data provided by Fassett, originally reported in Patty's 2nd edition, 1963. 6 hour LC50 0.41-2.22 mg/l. All rats died within 2 days at 2.22 mg/l while all survived at 0.41 mg/l. Concentrations calculated. No further details available. Data is reported in Iuclid 2000 and Opdyke, 1978.

**Test substance:** Isomer content and purity not reported.

**Reliability:** (4) not assignable
Secondary reference.

06-AUG-2005 (50) (66) (67)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Report of unpublished data. Rabbit LD50 >5000 mg/kg. No further details available. Study reported in Iuclid 2000.
**Reliability:** (4) not assignable
Secondary reference.
18-OCT-2004 (50) (66)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
18-OCT-2004

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** other: New Zealand White rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** water
**PDII:** 0
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Erythema (grade 1) observed at 1 hour after removal of dressings. All scores at other time points 0.
- Oedema: No oedema observed.

REVERSIBILITY: Initial erythema regressed in the first 24 hours. All scores at 24, 48 and 72 hours were 0.

OTHER EFFECTS: None reported.
**Source:** Sanders 1996b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: 2 male, 1 female
- Source: David Percival, Cheshire, UK
- Age: 12 -16 weeks
- Weight at study initiation: 2.36 - 2.54 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: The test material was a white solid, the test site was moistened with 0.5 ml purified water prior to application of 0.5 g of the solid.

- Area of exposure: 2.5 x 2.5 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 16 days
- Controls: Not rpeorted.
- Removal of test substance: Gentle swabbing with cotton.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours post application.

**Test substance:** Tradename Kalcol 6098
**Conclusion:** Following a 4 hour semi-occlusive exposure of Kalcol 6098 to rabbit skin there was no evidence of skin irritation between 24 and 72 hours after patch removal. Kalcol 6098 is not a skin irritant according to EU or GHs criteria.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
03-JAN-2006 (73)

**Species:** rabbit
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 9
**Vehicle:** petrolatum
**Result:** slightly irritating

**Method:** other
**Year:** 1972
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of unpublished data submitted to CTFA in 1972. Test volume 0.1 ml (50% in petrolatum). The test substance produced minimal to slight irritation. The author reports that identical results were obtained in a similar study.

This data is reported in other secondary references, Iuclid, 2000; Patty 2001,
**Source:** CIR, 1988
Hayes Consultancy Service Bromley, Kent
**Reliability:** (4) not assignable
Secondary reference.
25-JAN-2005 (16) (50) (67)

**Remark:** Secondary references to unpublished data reported in Patty 1963 cited by Opdyke, 1978, RTECS 2004 and Iuclid, 2000.

Guinea pig undiluted material produced only a mild effect.
**Test substance:** Cetyl alcohol, described in Patty, 1963 as a synthetic liquid C16 alcohol that may have contained impurities.
**Reliability:** (4) not assignable
Secondary reference.
06-AUG-2005 (50) (66) (68) (70)

**Remark:** Unpublished data reported to CFTA 1976

Hexadecyl alcohol tested at 12% in petrolatum produced no irritation in human subjects (Epstein 1976).

Undiluted cetyl alcohol applied undiluted to intact and abraded rabbit skin in a 24 hour occlusive exposure was described as non-irritant (Levenstein, 1976).

**Test substance:** Hexadecanol

**Reliability:** (4) not assignable
Secondary reference.

25-JAN-2005 (50) (66)

**Remark:** Secondary report in RTECS and IUCLID 2000 of a human skin test in which 75 mg of test substance was applied to the skin for 3 days. the reaction is described as mild. The data was originally reported in Cutaneous Toxicity, Proceedings of the 3rd Conference 1976. Drill & Lazar (eds.)

**Test substance:** Hexadecanol

**Reliability:** (4) not assignable
Secondary reference.

18-JAN-2006 (50) (70)

**Result:** Cetyl alcohol gave a low irritancy score in the closed patch test regardless of concentration. An increase in degree of irritancy with concentration was seen using the nitrocellulose replica method.

**Test condition:** Comparison of two methods of assessing skin irritation in man using a group of 20 healthy volunteers (aged 26-29 years). Each test compound was adjusted to a molar concentration in the range 0.5 - 2 m.

Closed patch test: 15 ul of the test compound in petrolatum was applied to a filter disk fitted to a Finn chamber and applied to the skin of the upper back for 24 hours using Scanpor tape. The test site was scored visually for erythema at 1 and 24 hours after removal of the patch.

Nitrocellulose replica method: The test material was applied in petrolatum to the flexor side of ht eforearm using a semi-open 24 hour application. 30 minutes after removal a visual assessment was made and a replica of the skin surface was made using nitrocellulose disks. These disks were removed after 1-2 minutes and examined microscopically.

**Test substance:** Cetyl alcohol 96% pure, isomeric content not reported.

**Reliability:** (2) valid with restrictions
Comparative screening study, well documented, meets generally accepted scientific principles, acceptable for assessment.

06-AUG-2005 (75)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand White rabbit

**Concentration:** undiluted

**Dose:** .1 ml

**Comment:** not rinsed

**No. of Animals:** 3
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores 0.3, 0, 0 (group mean score 0.1)
- Iris: 0
- Conjunctivae (Redness): All 0.3 (group mean score 0.3)
- Conjunctivae (Chemosis): 0, 0.3, 0.3 (group mean score 0.2)
- Overall irritation score: Maximum group mean score 15.3 at 1 hour post instillation. Classified as a mild irritant according to a modified Kay and Calandra system.

DESCRIPTION OF LESIONS: Dulling of the cornea noted in 2 animals 1 hour after instillation, diffuse corneal opacity noted in 1 rabbit at 24 hours post instillation. Iridial inflammation noted in 2 animals at 1 hour post instillation only. Moderate conjunctival irritation noted in all eyes at 1 hour which reduced to minimal conjunctival irritation at 24 hours.

REVERSIBILITY: All eyes were normal at 48 and 72 hours post instillation.

OTHER EFFECTS: Residual test material noted around the treated eyes at 1 hour post instillation.

**Source:** Sanders 1996g
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.69-3.01 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: White granular solid applied using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 78 mg)
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

**Test substance:** Tradename Kalcol 6098
**Conclusion:** Kalcol 6098 is not an eye irritant according to EU or GHS criteria.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
03-JAN-2006 (74)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** no data
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating

**Method:** Draize Test
**Year:** 1959
**GLP:** no data
**Test substance:** other TS: cetyl alcohol

**Remark:** Report of 2 similar unpublished studies carried out according to the Draize method 1959. Ocular irritation was scored at 1,2,3,4 and 7 days post instillation. An average score of 1 was reported on day 1 post instillation and signs of ocular irritation had cleared by day 2. In a second similar study the average score at day 1 was again 1 and all signs of irritation had cleared by day 2. Cetyl alcohol was considered at most minimally irritating in these tests. This study also appears to be reported in Iuclid 2000 and Patty, 2001.
**Test substance:** Cetyl alcohol (hexadecanol) isomer content not reported)
**Reliability:** (4) not assignable
Secondary reference some experimental detail provided.
03-JAN-2006 (16) (50) (67)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** other: albino Dunkin Hartley guinea pig
**Concentration 1st:** Induction 1 % intracutaneous
**2nd:** Induction 50 % occlusive epicutaneous
**3rd:** Challenge occlusive epicutaneous
**No. of Animals:** 15
**Vehicle:** other: arachis oil
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** OECD Guide-line 406 "Skin Sensitization"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: Intradermal. Erythema (grade 2) observed at all injection sites, no systemic toxicity. Tested at 1% only. Topical application for induction (48 hour) minimal irritation at 5 and 10%, with 25 and 50% maximum erythema score 2 persisting to 48 hours after removal of patch. Topical application for challenge initial minimal response at 1 hour, no irritation at 24 and 48 hours.

RESULTS OF TEST
- Sensitization reaction: No sensitisation reaction in any of the test or control animals. Response 0/10 test, 0/5 controls.
- Clinical signs: Body weights and weight gain over the observation period were comparable in test and control groups. One animal was killed after topical challenge, the reason was

not given but this was not considered to affect the results of the test. Well defined - moderate erythema at the intradermal injection site 24 hours after induction, well defined erythema at 48 hours. Following topical induction very slight to well defined erythema was noted 1 hour after patch removal, very slight erythema observed in 2/10 test animals at 24 hours. No skin reactions following topical challenge.
- Rechallenge: Not required.

**Source:** Driscoll 1996a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pigs
- Strain: Dunkin Hartley
- Sex: male
- Source: David Hall, Staffs, UK
- Age: 8-12 weeks
- Weight at study initiation: 376 -454 g
- Number of animals: 10
- Controls: 5

ADMINISTRATION/EXPOSURE
- Study type: M&K maximisation procedure (adjuvant method)
- Preparation of test substance for induction: in arachis oil
- Induction schedule: Day 1 intradermal induction, day 7 topical induction (48 hours occlusive).
- Concentrations used for induction: intradermal 1% in arachis oil, topical 50% in arachis oil.
- Concentration in Freuds Complete Adjuvant (FCA): 1%
- Challenge schedule: Day 21 topical challenge (24 hours occlusive)
- Concentrations used for challenge: 25 and 50% in arachis oil.
- Rechallenge: No
- Positive control: Evidence of reaction of the strain of guinea pigs to known skin sensitisers over an appropriate period was provided.

EXAMINATIONS
- Grading system: Draize 0-4 scale for erythema and oedema.
- Pilot study: Topical (24 and 48 hour occlusive) applications were tested at 5, 10, 25 and 50%. Intradermal injection was carried out at 1% the maximum suitable concentration.

**Test substance:** Tradename Kalcol 6098

**Conclusion:** Kalcol 6098 is not a skin sensitiser in the guinea pig when tested using the Magnusson and Kligman maximisation assay.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

05-DEC-2005 (21)

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction 5 % intracutaneous
**2nd:** Induction 5 % occlusive epicutaneous
**3rd:** Challenge 25 % open epicutaneous
**No. of Animals:** 20
**Vehicle:** other: olive oil, vaseline or ethanol
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: Magnusson & Kligman, 1969

**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF TEST
- Sensitization reaction: Response 0/20 test, 0/20 control
- Clinical signs: None
- Rechallenge: Not required

**Test condition:** TEST ANIMALS: Guinea pigs
- Strain: Pirbright white
- Sex: no data
- Source: no data
- Weight at study initiation: 400 - 500g
- Number of animals: 20
- Controls: 20

ADMINISTRATION/EXPOSURE
- Study type: adjuvant
- Preparation of test substance for intradermal induction: 5% in olive oil
- Preparation of test substance for topical induction: 5% in vaseline
- Induction schedule: 6 intracutaneous injections and patch tests. As described by Magnusson & Kligman, 1969.
- Concentration in Freuds Complete Adjuvant (FCA): 1:1
- Challenge schedule: As described by Magnusson & Kligman, 1969
- Concentrations used for challenge: 25% in vaseline or ethanol.
- Rechallenge: no
- Positive control: Not reported.

**Conclusion:** 1-hexadecanol is not a skin sensitiser when tested using the M&K maximisation procedure. Results cited in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
05-DEC-2005 (33) (50)

**Remark:** Secondary report of unpublished data. A maximisation test was carried out on 26 human volunteers with hexadecanol at a concentration of 12% in petrolatum. There were no sensitisation reactions.

The same Iuclid 2000 record reports a case of urticaria-like dermatitis in a 28 year old white female. No further details available.
**Test substance:** as prescribed by 1.1 - 1.4
**Reliability:** (4) not assignable
Secondary reference.
05-DEC-2005 (50) (66) (68)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-acute
**Species:** rat **Sex:** male/female
**Strain:** Sprague-Dawley
**Route of administration:** gavage

**Exposure period:** 28 days
**Frequency of treatment:** daily, 5 days/week
**Post exposure period:** 28 days
**Doses:** 100, 500, and 1000 mg/kg bw
**Control Group:** yes, concurrent vehicle
**NOAEL:** > 1000 mg/kg bw

**Method:** other: similar to OECD Guide-line 407
**Year:** 1985
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: >1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0, 100, 500 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: Unremarkable other than top dose females appearing rather defensive when handled.
- Body weight gain: Comparable with controls.
- Food and water consumption: Similar to control group
- Ophthalmoscopic examination: Comparable in treated and control animals.

- Clinical chemistry: Statistically significant changes (*95% ** 99% confidence) in some clinical chemical parameters were noted as follows:
500 mg/kg/day males increased potassium*, 500 mg/kg/day females increased GGT*, cholesterol** and chloride*. Glucose was elevated in top dose males (1000 mg/kg/day)**. These changes were not dose and/or sex related and not correlated with any histopathological findings and are therefore not considered of toxicological significance.

Serum glucose mmol/l:

| Control | Low | Mid | High |
|---|---|---|---|
| 6.03 | 6.20 | 6.25 | 7.28** |

- Haematology: No differences between treated and control animals other than an increase in neutrophils containing rodlike bodies observed in top dose females (confidence level 95%*). Values obtained (% rod like cells) were controls 2.5, low dose 3.3, mid dose 2.9, high dose 5.3*.

- Organ weights: Both absolute and relative organ weights were essentially comparable in treated and control animals. Sporadic changes were observed as follows (*95% ** 99% confidence) increases in absolute organ weight male kidney 500 mg/kg/day*, male testes 1000 mg/kg/day*. The only change in relative organ weight was an increase in male adrenal weight at 1000 mg/kg/day*.

Testes weight mean relative (absolute):

| Control | Low | Mid | High |
|---|---|---|---|
| 0.856 (3.207) | 0.839 (3.186) | 0.908 (3.455) | 0.893 (3.474)* |

Adrenal weight mean relative (absolute)

| | |
|---|---|
| | Control Low Mid High<br>0.013 0.014 0.014 0.015*<br>(0.050) (0.054) (0.055) (0.058)<br><br>- Gross and Histopathology: No treatment related histopathological changes in test, control or reversibility groups. |
| **Source:** | Henkel KGaA 1985a (in German); Henkel 1999 (a 1-page English summary). |
| | Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS<br>- Age/Weight at study initiation: M 84-98 g; F 81-93g<br>- Number of animals: 10M+10F per dose level plus 5M+5F per dose level for reversibility.<br><br>ADMINISTRATION / EXPOSURE<br>- Duration of test/exposure: 27-28 days exposure (5 days/week)<br>- Type of exposure: oral gavage<br>- Post exposure period: 28 days<br>- Vehicle: Olive oil<br>- Concentration in vehicle: 0, 2, 10 or 20%<br>- Total volume applied: 5 ml/kg<br>- Doses: 0, 100, 500 and 1000 mg/kg/day<br><br>SATELLITE GROUPS AND REASONS THEY WERE ADDED: 5M+5F per dose level for reversibility.<br><br>CLINICAL OBSERVATIONS AND FREQUENCY:<br>- Clinical signs: Daily<br>- Mortality: Daily<br>- Body weight: Weekly<br>- Food consumption: Daily<br>- Water consumption: Weekly<br>- Ophthalmoscopic examination: At end of study<br>- Haematology: After 21/22 daily doses: Haematocrit, MCV, Hb, RBC, WBC, Thrombocytes, differential white count.<br>- Biochemistry: After 21/22 daily doses: Serum Urea, creatinine, Na, K, calcium, alkaline phosphatase, ALAT, ASAT, GT, bilirubin, chloride, albumin, total protein, chloesterol.<br>- Urinalysis: Not done<br><br>ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):<br>- Macroscopic: Yes<br>- Organs weights: thyroid, adrenals, thymus, kidney, spleen, heart, brain, testes, liver.<br>- Microscopic: All organs from the control and top dose animals were examined plus the animals from the reversibility study.<br><br>STATISTICAL METHODS: T-test. U-test for organ weights. |
| **Test substance:** | Tradename Lanette 16 |
| **Conclusion:** | NOAEL is considered to be >1000 mg/kg/day based on lack of toxicologically significant treatment related effects at this dose level (top dose level). Sporadic statistically significant changes in some organ weights and clinical chemical parameters were observed but these were not associated with histopathological changes and were not considered of toxicological significance. |

This study is also reported in summary in Iuclid 2000 for hexadecanol.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Report in German language, English summary page.

**Flag:** Critical study for SIDS endpoint

03-JAN-2006 (41) (43)

**Type:** Sub-chronic
**Species:** other: Albino rats **Sex:** male/female
**Strain:** other: ex Charles River
**Route of administration:** oral feed
**Exposure period:** 13 weeks
**Frequency of treatment:** Daily
**Post exposure period:** none
**Doses:** 1% and 2.5% for 13 weeks, 5% for 10 weeks then 7.5% (week 11) and 10.0 % (weeks 12 & 13).
**Control Group:** yes
**NOAEL:** = 723 mg/kg bw

**Method:** other: see text
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).
**Result:** NOAEL: M 723 mg/kg/day F 875 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
1%: M 723 mg/kg/day; F875 mg/kg/day
2.5%: M1822 mg/kg, day; F 2064 mg/kg/day
5%: M 4257 mg/kg/day; F4567 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: All animals survived the 13 week treatment period.

- Clinical signs: all surviving animals appeared normal.

- Body weight: Significantly reduced (84.7 - 89.8% of controls) in top dose males for most study weeks, in mid dose females at weeks 4-13 and high dose females (81.7-89.7%) throughout the study. Changes were attributed at least in part to reduced food consumption and the high content of test material in the diet.

- Food consumption: Significantly reduced (76.4 - 89.2% of controls) in top dose males at weeks 1 and 12, in mid dose males at week 13, in mid dose females at week 1 and high dose females weeks 1 and 12 (79.1 - 89.9% of controls).

- Clinical chemistry: not carried out.
- Haematology: no treatment related changes.
- Urinalysis: no treatment related changes.

- Organ weights: The original report indicates that there were significant differences in some relative organ weights from treated groups compared to controls. These were reanalysed by the Weinberg Group using the Tukey test. The significant

changes found in the original report together with the results of the Weinberg analysis are summarised below.

| Organ | Sex | Orig. sig. at | Weinberg report |
|---|---|---|---|
| Brain | M | low-dose | Not significant |
| | M | high-dose | Significant |
| | F | mid dose | Significant |
| | F | high-dose | Significant |
| Heart | M | high-dose | Significant |
| | F | high-dose | Not significant |
| Liver | M | mid dose | Not significant |
| | M | high-dose | Significant |
| | F | low-dose | Not significant |
| | F | mid dose | Not significant |
| | F | high-dose | Significant |
| Spleen | F | mid dose | Not significant |
| | F | high-dose | Significant |
| Gonad | M | low-dose | Not significant |
| | M | high-dose | Significant |

Additionally Weinberg reanalysed the organ weight data for the kidney and adrenal and thyroid which showed no significant changes from the original statistical analysis. The thyroid weight showed a significant increase in mid dose males only according to the Weinberg analysis.

Statistical results are not reported in detail, while individual animal data are reported means are not given. Using this data to calculate the mean and SD for the organ weight changes originally reported as significant (see table above) the magnitude of the changes is a follows:

Brain weight mean relative:

| | Control | Low | Mid | High | |
|---|---|---|---|---|---|
| Males | 0.454 | | 0.486* | 0.497 | 0.523*+ |
| SD | 0.01 | 0.029 | 0.072 | 0.03 | |
| Female | 0.646 | | 0.692 | 0.795*+ | 0.797*+ |
| SD | 0.066 | | 0.021 | 0.004 | 0.01 |

Heart weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 0.296 | 0.286 | 0.323 | 0.293* |
| SD | 0.005 | 0.028 | 0.039 | 0.014 |
| Female | 0.305 | 0.315 | 0.329 | 0.392*+ |
| SD | 0.023 | 0.008 | 0.054 | 0.025 |

Liver weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 3.029 | 3.168 | 3.09* | 3.756*+ |
| SD | 0.302 | 0.021 | 0.653 | 0.361 |
| Female | 3.466 | 3.549* | 3.55*+ | 3.659* |
| SD | 0.198 | 0.139 | 0.008 | 0.275 |

Spleen weight mean relative:

| | Control | Low | Mid | High | |
|---|---|---|---|---|---|
| Female | 0.189 | | 0.205 | 0.212* | 0.233*+ |

SD 0.018 0.025 0.009 0.065

Gonad weight mean relative:

| | Control | Low | Mid | High |
|---|---|---|---|---|
| Males | 0.793 | 0.768* | 0.787 | 0.902*+ |
| SD | 0.062 | 0.003 | 0.084 | 0.052 |

*Significant using Chi square test as reported in original report. +Significant in Tukey test.

- Gross pathology: Unremarkable
- Histopathology: There were no treatment related histopathological changes in the control and top dose animals examined (including testes & ovaries).

STATISTICAL RESULTS: Original organ weight analyses using the Chi square test were supplemented by Tukey tests carried out by the Weinberg group.

**Source:** Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: Actual age not reported, described as young.
- Weight at study initiation: M 103.8 g; F 90.4 g
- Number of animals: 10M + 10F per test group, 20M + 20 F controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 13 weeks
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 1.0, 2.5 and 5% in the diet. The 5% dose was increased to 7.5% in week 11 and 10% in weeks 12 and 13.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily (5 days/week)
- Mortality: Daily (5 days/week)
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: Not carried out.
- Haematology: At 30 days and 90 days on 5M+5F. Micro haematocrit, Hb, total & differential leucocytes.
- Biochemistry: Not carried out.
- Urinalysis: At 30 days and 90 days on pooled samples from 5 rats of each sex.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Complete necropsy performed, organ weights measured were brain, thyroid, heart, liver, spleen, kidneys, adrenals, ovaries & testes.
- Microscopic: Tissues fixed: brain, thyroid, parathyroid, heart, lung, liver, spleen, stomach, small & large intestine, pancreas, kidney, urinary bladder, adrenals, ovaries, testes, lymph node, bone, bone marrow, muscle. All tissues from 5M+5F high dose and control animals were examined.

STATISTICAL METHODS: The original report indicates that a Chi square test was carried out on the organ:bodyweight ratio. It is not clear what statistical methods were used (if they were)

for body weights, food consumption & haematological parameters. Subsequently The Weinberg Group Inc. used Tukeys test to re-analyse the organ weight data.

**Test substance:** Tradename Alfol 16

**Conclusion:** The NOAEL for this 13 week dietary feeding study in rats is ca 750 mg/kg/day (males 723, females 875) based on reduced weight gain and food consumption. The toxicological significance of observed changes in organ weights, all in the absence of histopathological change, is questionable. Increased liver weights at higher dose levels may be indicative of a mild adaptive effect on the liver.
This study was also reported in summary in Iuclid 2000 for hexadecanol.

**Reliability:** (2) valid with restrictions
Valid with restrictions including lack of biochemical investigations and limited reporting of statistical findings. Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

03-JAN-2006 (50) (77)

**Type:** Sub-chronic
**Species:** dog **Sex:** male/female
**Strain:** Beagle
**Route of administration:** oral feed
**Exposure period:** 13 weeks
**Frequency of treatment:** daily
**Post exposure period:** none
**Doses:** 0.5, 1.0, and 3.0 % w/w
**Control Group:** yes, concurrent no treatment
**NOAEL:** > 1054 mg/kg bw

**Method:** other: (see text)
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).

**Result:** NOAEL (NOEL): M 1175 mg/kg/day; F 1054 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0.5% (M 208 mg/kg/day; F 186 mg/kd/day)
1% (M 502 mg/kg/day; F 374 mg/kg/day)
3% (M 1175 mg/kg/day; F 1054 mg/kg/day)

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No animals died.
- Clinical signs: No specific clinical signs, all animals appeared normal and healthy throughout the study. This was suppported by the clinical examinations at weeks 3, 6 and 13 which were within normal limits.
- Body weight gain: Comparable in test and control groups.
- Food/water consumption: Comparable in test and control groups.
- Ophthalmoscopic examination: Not carried out.
- Clinical chemistry: No treatment related adverse effects for most parameters. Plasma ALAT levels were increased at all dose levels at 13 weeks only.
- Haematology: No adverse effects.

- Urinalysis: No adverse effects.
- Organ weights: These were within normal limits and comparable to controls. Tukeys test did not indicate any statistical differences (however sample size was small).
- Gross pathology: Lymph node hyperplasia in both control and treated animals was considered due to roundworm infestation (despite routine deworming throughout the study). There were no treatment related findings.
- Histopathology: No treatment related changes.
- Other: ECG's showed no difference between the initial pattern recorded pretreatment and those seen at 3 and 13 weeks.

STATISTICAL RESULTS: There was no statistical analysis of the study data in the original report. Subsequent analysis of organ weights using Tukeys test did not reveal any statistical differences between treated and control animals. This analysis was carried out by The Weinberg Group Inc.

**Source:** Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 5 months
- Weight at study initiation: M4.77-8.63 kg; F5.45-7.49 kg
- Number of animals: 2M+2F treated; 4M+5F controls

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 13 weeks
- Type of exposure: dietary
- Post exposure period: None
- Vehicle: Diet
- Doses: 0.5, 1% and 3% in diet

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily 5 days/week. Complete physical examination, body temperature, pulse rate, reflexes, mucous membranes, auscultation pretreatment at 3, 6 & 13 weeks. ECG pretreatment, 3 and 13 weeks.
- Mortality: Daily
- Body weight: weekly
- Food consumption: weekly
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Not recorded.
- Haematology: Total & differential leucocyte counts, Hb, haematocrit, erythrocyte sedimentation rate, prothrombin time measured pretreatmentand at 3, 6 and 13 weeks.
- Biochemistry: Plasma levels of glucose, total protein & albumin, albumin/globulin ratios, urea nitrogen measured pretreatment, 3, 6 and 13 weeks. Liver function assessed by BSP retention, alkaline phosphatase & SGOT at same time periods.
- Urinalysis: albumin, glucose, bilirubin, pH, vol. , specific gravity, microscopic examination of sediment, total nitrogen. Carried out pretreatemnt & at 3, 6 & 13 weeks.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: complete, organ weights determined for brain, thyroid, heart, liver, kidneys, adrenals, spleen, gonads.
- Microscopic: Brain, pituitary, sub-maxillary salivary gland, thyroid, parathyroid, heart, lung, liver, spleen, stomach (fundic & pyloric), small intestine (3 levels), large

intestine, pancreas, gall bladder, kidney, urinary bladder, adrenal, gonads, lymph node (cervical & mesenteric), bone, bone marrow, muscle (striated). All fixed. Tissues from controls & high dose animals examined microscopically. Stomach & intestinal tissues from mid dose animals also examined plus any abnormal tissues identified at necropsy.
STATISTICAL METHODS: No statistical analysis reported in the original report. For the HPV program the results were analysed using Tukey's Test.

**Test substance:** This substance corresponds to CAS# 36653-82-4. Tradename is Alfol 16. Described as a white, wax-like solid. No other analytical details.
Tradename Alfol 16

**Conclusion:** The NOAEL for Alfol 16 following dietary administration is considered to be >1175 mg/kg/day for male dogs and >1054 mg/kg/day for females. This was the highest dose level tested (3% in diet). The elevated ALAT values seen at 13 weeks in most test animals at all dose levels were apparently not dose related or accompanied by histopathological liver change. Other markers of liver function appeared normal. This study was also reported in summary in Iuclid 2000 for hexadecanol.

**Reliability:** (2) valid with restrictions
Reliability 2 however there were methodological deficiencies, animal group size too small (2M + 2F in test groups), no statistical analysis in original study, subsequent analysis by The Weinberg Group Inc of limited relevance because of small group sizes.

03-JAN-2006 (50) (78)

**Type:** Sub-acute
**Species:** rat **Sex:** male
**Strain:** Wistar
**Route of administration:** oral feed
**Exposure period:** 12 days
**Doses:** 5% (50000 ppm)
**Control Group:** yes, concurrent no treatment

**Method:** other
**Year:** 1971
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This study was undertaken to evaluate the available energy provided by cetyl alcohol and other alcohols, acids, esters and carbonyl substances in the diet. Cetyl alcohol at a concentration of 5% in the diet was administered over a 12 day period to 8 rats. All rats administered cetyl alcohol in the diet at 5% died within the 12 days.

**Test substance:** Described as cetyl alcohol no detail of purity or isomeric content.

**Reliability:** (3) invalid
As all the rats died little information can be drawn from this study.

06-AUG-2005 (105)

**Remark:** Summary report from NTIS publication (not available). Repeated oral administration to dogs of 91 g/kg over a 12 week period resulted in tremors, ataxia and death. No further details available.

**Test substance:** hexadecanol, no further information
**Reliability:** (4) not assignable
Secondary reference.
06-AUG-2005 (71)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Bacterial reverse mutation assay
**System of testing:** Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
**Concentration:** 50 to 5000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: 5000 ug/plate this did not interfere with counting revertant colonies.

CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.
**Source:** Thompson 1996c.

Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced

ADMINISTRATION:
- Dosing: 50, 150, 500, 1500 and 5000 ug/plate for both tests.
- Number of replicates: Duplicate tests each performed in triplicate
- Application: Plate incorporation assay, vehicle acetone
- Positive and negative control groups and treatment: Vehicle control- acetone. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and

statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to controls.
**Test substance:** Tradename Kalcol 6098
**Conclusion:** The C16 alcohol Kahlcol 6098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (88)

**Type:** other: Bacterial reverse mutation assay screening test
**System of testing:** Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538
**Concentration:** 50 ug/spot
**Cytotoxic Concentration:** 50 ug/spot
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: Ames et al. 1975.
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No evidence of increased reverse mutation in any strain in this screening (spot) test. Appropriate responses were obtained with positive and negative controls.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: By inference a non-cytotoxic concentration (50 ug/spot) was chosen for this screening test.
**Source:** Blevins and Taylor 1982.

Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: Spot test at a single concentration of 50 ug.
- Number of replicates: Not replicated, screening test only.
- Application: Spot test assay, vehicle sterile double distilled water.
- Positive and negative control groups and treatment: Vehicle control and 2-aminoanthracene to demonstrate activity of the S9 metabolising fraction. No other positive controls.
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Increase in revertants over control levels, however further details were not reported.

**Conclusion:** Hexadecanol was evaluated in a screening test using histidine deficient strains of Salmonella typhimurium. There was no evidence of mutagenic activity with or without metabolising fraction. Results also reported in summary in CIR 1988.
**Reliability:** (4) not assignable
Comparative screenng study only.
11-MAY-2006 (12)

**Type:** other: Bacterial reverse mutation assay (Ames Test)
**System of testing:** Salmonella typhimurium strains TA 100, TA 1535, TA 1537, TA 1538, TA 98
**Concentration:** 4, 20, 100, 500, 2500 ug/plate
**Cytotoxic Concentration:** Not cytotoxic without S9, some evidence of cytotoxicity with S9 at 500 and/or 2500 ug/plate.
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: An in-house protocol based on OECD Guide-line 471
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls gave an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Some evidence of a decrease in revertants at higher dose levels for TA 100 and TA 1535, effect on background lawn not reported.
- Without metabolic activation: No clear cytotoxic effect.

**Source:** Henkel KGaA 1981d.
Hayes Consultancy Service Bromley, Kent
**Test condition:** METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls. no repeat assay.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Duplicate.
- Application: Plate incorporation, aqueous suspension with Tween 80.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

**Test substance:** Tradename Lanette 16

**Conclusion:** The C16 alcohol Lanette 16 (Lorol 16) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. There was some evidence of cytotoxicity in some strains at higher dose levels (500 and/or 2500 ug/plate) in the absence of metabolising fraction. This study was also reported in summary in the Iuclid 2000 for hexadecanol.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (40) (50)

## 5.6 Genetic Toxicity 'in Vivo'

**Type:** Cytogenetic assay
**Species:** rat **Sex:** male
**Strain:** other: unspecified
**Route of admin.:** other: intragastric
**Exposure period:** 48 hours
**Doses:** 1/5th LD50
**Result:** ambiguous

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:

600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 2.8 +-0.7
Cells with breakages %: controls 0.3 +-0.2; treated 0.4 +-0.2;
Cells with chromosome aberrations %: controls 0; treated 2.8 +-0.7.

STATISTICAL RESULTS: Reported as above.

**Test condition:** TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage
- Vehicle: Homogenised emulsion

- Duration of test: 48 hours
- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Conclusion:** Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability:** (3) invalid
Significant methodological deficiences (see test conditions).

19-OCT-2004 (10)

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (80) (81) (94)

## 5.7 Carcinogenicity

**Species:** mouse **Sex:** female
**Strain:** Swiss
**Route of administration:** dermal
**Exposure period:** 60 weeks
**Frequency of treatment:** three times weekly
**Post exposure period:** none
**Doses:** 4 ug/mouse in cyclohexane
**Result:** negative
**Control Group:** no

**Method:** other: skin tumour promotion study
**Year:** 1966
**GLP:** no data
**Test substance:** other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.
**Source:** Sice 1966.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane

- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)
- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Test substance:** The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Conclusion:** In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999). Results are also reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

19-OCT-2004 (9) (50) (62) (63) (79)

**Species:** mouse **Sex:** no data
**Strain:** other: Swiss albino ddY
**Route of administration:** i.p.
**Exposure period:** 5 days
**Frequency of treatment:** daily
**Post exposure period:** 24 days
**Doses:** Test 1: 2.5 or 10 mg/mouse/day. Test 2: 2, 4 or 8 mg/mouse/day 2.5 and 10 mg/mouse/day for C16 & 18 alcohols.
**Result:** negative
**Control Group:** yes

**Method:** other: determination of antitumour activity against Ehrlichs Ascites Tumour
**Year:** 1972
**GLP:** no
**Test substance:** other TS: other TS: Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Result:** The C10, 12, and 14 alcohols exhibited toxicity to the mice, evidenced by severe diarrhoea and loss of body weight. The dose levels were reduced in the repeat test. The mean survival

time for the untreated control group (Ascites implantation only) was 18.3 days in test1 and 14.4 days in test 2. All of the alkanols tested increased the survival time of mice implanted with ascites tumour cells at one or more dose levels tested. Life span was prolonged by 124 - >194%.

**Source:** Ando et al, 1972
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS Mouse Swiss albino ddY implanted ip with ascites tumour cells.
- Age: 5 weeks
- Weight at study initiation: 20-23g
- Number of animals: 4 or 6/ treatment group, 20 controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 5 days starting 24 hours afeter implantation of the ascites tumour cells.
- Type of exposure: Intraperitoneal
- Post exposure period: 24 days
- Vehicle: Probably aqueous suspension using Tween 80.
- Concentration in vehicle: Not reported.
- Doses: Test 1: for all 5 alcohols tested dose levels were 2.5 and 10 mg/mouse. Test 2: C10, 12 and 14 alcohols were tested at 2, 4 and 8 mg/mouse, C16 and 18 alcohols were tested at 2.5 and 10 mg/mouse.

OBSERVATIONS
The mean survival time was recorded and compared to the untreated control group.

**Conclusion:** Treatment with C10 -18 alcohols extended the survival time of mice implanted intraperitoneally with Ehrlich ascites tumour cells.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

31-AUG-2004 (2)

## 5.8.1 Toxicity to Fertility

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** rat
**Sex:** male/female
**Strain:** other: Charles river
**Route of administration:** oral feed
**Exposure Period:** 13 weeks
**Frequency of treatment:** continuous
**Duration of test:** 13 weeks
**Doses:** 1.0% and 2.5% for 13 weeks, 5.0% for 10 weeks then 7.5% week 11 and 10.0% weeks 12 & 13.
**Control Group:** yes
**NOAEL Parental:** = 1822 mg/kg bw

**Method:** other
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).

**Result:** None of the animals displayed overt signs of intoxication due

to oral exposure to hexadecanol during the 13 weeks of the experiment. Food consumption and body weights differed significantly for both males and females at various times in the intermediate and high dose levels. The relative testes weights were increased over control levels in all treatment groups reaching signficance in the low and high group according to the study report. The organ weight data were reanalysed by the Weinberg Associates using a Tukey test when significance was attained only at the high dose level. There were no significant changes in ovary weight. Histopathological examination revealed no treatment related changes in the ovaries or testes. The NOAEL for effects on the male reproductive organs can be considered as a dietary concentration of 2.5% (ca 2000 mg/kg/day) the NOAEL for the female reproductive organs is the highest dose level (ca 4000 mg/kg/day). Actual dose levels achieved at respective NOAELs, males 1822 mg/kg/day and females 4567 mg/kg/day. Full study report is to be found in Chapter 5.4 Repeated dose toxicity.

**Source:** Scientific Associates, Inc. 1966a.

Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 20 rats (10 of each sex) were fed Alfol 16 in the diet for 13 weeks. The control group consisted of 20 males and 20 females at dose levels of 1, 2.5 and 5% with the top dose level increasing at week 11 to 7.5% and for weeks 12& 13 to 10% in the diet. At termination, all animals were necropsied and tissues from 5 males and 5 females (including gonads) of the high dose group and a similar number of controls were examined histopathologically. Testes and ovary weights were recorded together with other organ weights. For full experimental details see Chapter 5.4 Repeat dose toxicity.

**Test substance:** Tradename Alfol 16

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

06-AUG-2005 (77)

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** dog
**Sex:** male/female
**Strain:** Beagle
**Route of administration:** oral feed
**Exposure Period:** 13 weeks
**Frequency of treatment:** daily
**Duration of test:** 13 weeks
**Doses:** 0.5, 1.0 and 3.0% w/w
**Control Group:** yes
**NOAEL Parental:** > 1054 mg/kg bw

**Method:** other
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** These results were reported to USEPA in accordance with TSCA 8(e).

**Result:** There were no overt signs of toxcity and no treatment related histopathological changes. There were no adverse effects on male or female reproductive organs as evidenced by lack of effect on gonad weights and lack of histopathological changes

in the gonads of the high dose animals. The value of this study is limited by the small numbers of animals used.

**Source:** Scientific Associates, Inc. 1966b.

Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of beagle dogs (2 of each sex/dose level) were exposed to hexanol at dose levels of 0.5, 1.0% and 3% w/w in the diet for 13 weeks. The control group contained 4 males and 5 females. Full details of this study are reported in Chapter 5.4 Repeat dose toxicity. Testes and ovaries were weighed and organs from top dose dogs examined histopathologically.

**Test substance:** Tradename Alfol 16

**Conclusion:** The NOAEL for effects on the reproductive organs of dogs is >1054 mg/kg/day (3% in the diet). There were no treatment related effects on reproductive organ weights and no histopathological changes in the gonads of top dose animals. This is also the NOAEL for systemic toxicity.

**Reliability:** (2) valid with restrictions
Reliability 2 however there were methodological deficiencies, animal group size too small (2M + 2F in test groups), no statistical analysis in original study, subsequent analysis by The Weinberg Group Inc of limited relevance because of small group sizes.

06-AUG-2005 (78)

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** rat
**Sex:** male/female
**Strain:** Sprague-Dawley
**Route of administration:** gavage
**Exposure Period:** 28 days
**Frequency of treatment:** daily
**Duration of test:** 28 days
**Doses:** 100, 500, and 1000 mg/kg bw
**Control Group:** yes
**NOAEL Parental:** = 1000 mg/kg bw

**Method:** other: An in-house protocol based on OECD Guide-line 407
**Year:** 1985
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were no deaths among the test animals. Food intake, water consumption, body weight, organ weight, and haematological parameters were not affected.
The absolute and relative organ weights of the ovary and testes were determined and were comparable to controls.
Reproductive tissues from the control and top dose animals (1000 mg/kg/day were examined histopathologically. In females examination of the ovaries, uterus and vagina and in males histopathological examination of the testes and prostate showed no difference between treated and control groups. The NOAEL for effects on the reproductive organs was considered to be 1000 mg/kg/day.

**Source:** Henkel KGaA 1999 (English summary); Henkel 1985a is the original report in German
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 10M+10F rats received daily doses of 0, 100, 500 and 1000 mg/kd Lanette 16 by gavage for 28 days. Full details of

this study are reported in Chapter 5.4 Repeated dose toxicity. The testes and ovaries were weighed and these organs plus the prostate, uterus and vagina from all control and top dose animals were subject to histopathological examination.

**Test substance:** Tradename Lanette 16

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

06-AUG-2005 (41)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that hexadecanol is not expected to be a developmental toxicant in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

25-OCT-2005 (80) (81) (94)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: development of skin irritation test

**Remark:** The purpose of this study was to introduce the chamber-scarification test designed for increased sensitivity for assessing the irritancy of materials. It is important to note that persons especially vulnerable to irritants were selected.

The materials were applied as a 25% solution in mineral oil. The skin is first scarified and the test material applied (0.1

ml) in a test chamber once daily for 3 days to groups of 5-10 volunteers. The skin was assessed 30 minutes after the end of the final exposure.

The degree of irritation was related to carbon chain length, the C10 and C12 alcohols giving a marked response while the C14 alcohol gave a moderate response, C16 slight and the oleyl alcohol gave a low response.

**Source:** Frosch & Kligman, 1976
Hayes Consultancy Service Bromley, Kent

**Test substance:** oleyl alchol, hexadecyl alcohol, tetradecyl alcohol, dodecyl alcohol, decyl alcohol

**Reliability:** (2) valid with restrictions

03-JAN-2005 (28)

**Type:** other: skin reaction in man

**Result:** Cetyl alcohol (C16) did not produce positive responses in any of the test subjects.

**Test condition:** Between May 1992 and September 1995 146 patients, of both sexes aged 13-72 years with suspected cosmetic or medicament contact dermatitis, were patch tested with a series of 5 fatty alcohols. Fatty alcohols >99% pure were used for the patch testing. The materials were applied (30% in petrolatum) to the skin for 2 days using Finn chambers on Scanpor tape. Readings were made at 2, 3 and 7 days. 108 females and 38 males were tested.

**Test substance:** Cetyl alcohol (1-hexadecanol 99% pure)

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

03-JAN-2005 (89)

**Type:** other: allergic skin reaction in man

**Remark:** The authors report the results of patch testing with aliphatic alcohols in 1664 consecutive patients at a dermatological clinic. Patch testing with cetyl alcohol (30% in vaseline) resulted in 2 positive reactions an incidence of 0.12%.
Cited in the Cosmetic Ingredient Review, 1985.

**Test substance:** Cetyl alcohol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

24-JAN-2005 (16) (45)

**Type:** other: allergic skin reaction in man

**Remark:** In a retrospective survey of allergic reactions to cosmetics, data on 475 patients with contact allergy to cosmetic ingredients were collected in 5 European dermatology centres. The observations were made over a 4 month period in 1996. A positive response to cetyl alcohol was obtained in only 3/475 patients.

**Test substance:** Cetyl alcohol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific

principles, acceptable for assessment.

24-JAN-2005 (34)

**Type:** other: allergic skin reaction in man

**Remark:** 9 patients with allergy to Lanette cream were tested with its consituents one of which is cetyl alcohol present at approximately 7%. All the patients showed positive reactions with 5% cetyl alcohol in petrolatum. These patients also reacted to Cetomacrogol cream, wood alcohols and/or lanolin. There was some discussion as to the correct test concentration for cetyl alcohol.
**Test substance:** Cetyl alcohol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
Summary report of case study.

24-JAN-2005 (93)

**Type:** other: allergic skin reaction in man

**Remark:** 330 patients with eczematous lesions were tested with a series of 27 topical substances including cetyl alcohol. Of these 330 there were 88 patients with leg ulcers. 21.6% of patients with leg ulcers reacted to cetyl alcohol (30% in white petrolatum) while 7.4% of non-ulcer patients also reacted. The higher than expected incidence of sensitisation reactions to cetyl alchol was attributed to the preferential choice of cetylic creams for outpatient use. The patients also gave positive reactions to other test substance including wool alcohols.

This reference was cited in CIR, 1988
**Test substance:** Cetyl alcohol
**Reliability:** (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.

24-JAN-2005 (13) (16)

**Type:** other: allergic skin reaction in man

**Remark:** 100 patients, with suspected allergic eczematous contact dermatitis due to topical medications, were patch tested with 15 different substances frequently found in the vehicles for topical medications. Cetyl alcohol tested at 30% in petrolatum did not produce any reaction.

Cited in CIR, 1988
**Test substance:** Cetyl alcohol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

25-JAN-2005 (16) (22)

**Type:** other: comparative skin irritation

**Result:** 2-hexadecyl alcohol was found to be severely irritating to the

skin of rabbits and rats, moderately irritating to guinea pig skin, mildly irritating to the skin of humans and non-irritating to the skin of minature swine.

This report is cited by Opdyke, 1978, RTECS 2004 and Iuclid, 2000 as referring to 1-hexadecanol but it is obvious from the original report that 2-hexadecanol was tested.

**Test condition:** Animal studies: albino angora rabbits ave wt. 2.6 kg, Hartley guinea pigs 350-500g and Wistar rats 250-350g. Groups of 6 animals received 0.1g of undiluted test material to the shorn dorsal skin. The test material was allowed to remain in contact with the skin for 24 hours, uncovered. After 24 hours the skin reactions were scored and a further identical application made. At 48 hours the sites were scored again and then at 72 hours. The animals were then injected intravenously with Evans Blue dye and an hour later they were sacrificed and the dorsal skin removed. Minature swine were also tested receiving a 48 hour patch test with 0.05g of test material. The test site was evaluated as described above.

The intact skin was scored for redness (72 hours) while the excised skin was assessed for the dilating rate of blood vessels, oedema, blueing rate (indication of increased capillary permeability) and the bleeding rate. Scores for the various parameters were combined to give a so called primary irritation index (total score). Total score = dilating rate + swelling rate + blueing rate + bleeding rate + reddening rate. Scores <= 4 indicated mild irritation, 4-8 moderate irritation and >8 severe irritation.
Histopathological examination of the skin was also carried out.

Human studies: 50 human volunteers received patches with 0.05 g of the test material, these remained in place on the back for 48 hours and scored 30 minutes after removal and then at up to 120 hours as necessary.

**Test substance:** 2-hexadecanol

**Reliability:** (2) valid with restrictions
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

25-JAN-2005 (50) (61) (66) (70)

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 143-28-2 |
| **CAS No.** | 143-28-2 |
| **EINECS Name** | (Z)-octadec-9-enol |
| **EC No.** | 205-597-3 |
| **Molecular Formula** | C18H36O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **08-MAR-2006** |
| **Number of Pages:** | **44** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

23-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** Cognis Deutschland GmbH
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** 26, V. Medici del Vascello
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
19-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinnati, OH
**Country:** United States

**Remark:** Consortium Member
19-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
03-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.
The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |

| | |
|---|---|
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 9-Octadecen-1-ol, (9Z)-
**Smiles Code:** OCCCCCCCCC=CCCCCCCCC
**Mol. Formula:** C18 H36 O1
**Mol. Weight:** 268.49
21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential.
Non-confidential data are summarised here.
Of the commercial products associated with the Consortium members, those identified as 9-Octadecen-1-ol, (9Z)-, CAS 143-28-2 are 100% linear.

The substance comprises >70% C16/18, <10% C14, including >70% C18 unsaturated. Components of even chain length, in the range C12-C20 are present.
05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required.
05-AUG-2005

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

9-Octadecen-1-ol, (9Z)- (9CI) (CA INDEX NAME)
9-Octadecen-1-ol, (Z)- (8CI)
Adol 85NF
Atalco O
Cachalot O 1
cis-.DELTA.9-Octadecenol
cis-9-Octadecen-1-ol
cis-9-Octadecenyl alcohol
Crodacol O
Dermaffine
HD-Eutanol
HD-Ocenol 90/95
HD-Ocenol 92/96
HD-Ocenol K
Loxanol 95
Loxanol M
Novol
Ocenol
Ocenol 90/95
Octadeca-9-cis-en-1-ol

Oleic alcohol
Oleo alcohol
Oleol
Oleyl alcohol
Rikacol 90BHR
Satol
Sipol O
Siponol OC
Unjecol 70N
Unjecol 90
Unjecol 90BHR
Unjecol 90N
Unjecol 90NR
Vegecol 90B
Witcohol 85NF
Witcohol 90NF
Oleyl Alcohol
(Z)-9-Octadecen-1-ol
(Z)-9-Octadecenol
9-cis-Octadecenol
Adol 320
Adol 330
Adol 80
Adol 85

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 9-octadecen-1-ol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >500 - 5 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to 1 000 000 - 10 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (6) (19) (27)

### 1.6.1 Labelling

-

### 1.6.2 Classification

-

### 1.6.3 Packaging

-

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.
The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site

limited).

21-DEC-2005

**Use category:** 5 Anti-freezing agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 38 Plant protection products, agricultural
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

-

## 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 658.
05-AUG-2005 (29)

### 1.8.4 Major Accident Hazards

-

### 1.8.5 Air Pollution

-

### 1.8.6 Listings e.g. Chemical Inventories

-

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 9-octadecen-1-ol. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

-

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
03-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-AUG-2005

## 2.1 Melting Point

**Value:** = 13 - 19 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised, peer-reviewed source
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (9)

## 2.2 Boiling Point

**Value:** = 333 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (22)

## 2.3 Density

**Value:** = .8489 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised, peer-reviewed source
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (18)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0000198 hPa at 25 degree C

**Method:** other (calculated): SRC MPBPVP v1.40
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Vapour pressures for branched components present in the substance, within the limits described in section 1.1-1.4, are expected to be in line with the linear alcohols of equivalent carbon number.

Validation of vapour pressure prediction using this method shows that the calculated values are likely to be reliable.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.

**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 7.07 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .042 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.042 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-SEP-2005 (1)

**2.6.2 Surface Tension**

-

**2.7 Flash Point**

-

**2.8 Auto Flammability**

-

**2.9 Flammability**

-

**2.10 Explosive Properties**

-

**2.11 Oxidizing Properties**

-

**2.12 Dissociation Constant**

-

**2.13 Viscosity**

-

**2.14 Additional Remarks**

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 79.71815E-12 cm3/molecule.sec
Half-life: 4.8 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Unsaturated components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than saturated components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
09-SEP-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 268.5
Data temperature 25 deg C
Log Kow 7.07
Water Solubility 0.0077 mg/l
Vapour pressure 0.00198 Pa
Melting point 17 deg C
half life in air 4.8 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 0.13% |
| Soil | 97.6% |
| Water | 9.38E-03% |
| Fish | 5.51E-03% |
| Sediment | 2.17% |

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 8.01 | 0.000579 | 9.86E-06 |
| % in water | 1.17 | 2.65 | 0.0105 |
| % in sediment | 42.9 | 97.3 | 0.383 |
| % in soil | 47.9 | 0.00347 | 99.6 |

The results reflect that the ultimate fate of 9Z-octadecen-1-ol is dependent on its route of release into the environment. 9Z-octadecen-1-ol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.In water, the adsorption coefficient of 9Z-octadecen-1-ol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The estimated log Kow value of 7.07 was used in the TGD calculation methods.

**Result:** TGD Hydrophobics method: Koc = 671000
TGD Non-hydrophobics method: Koc = 49700
TGD Alcohols method: Koc = 1810
SRC PCKOCWIN method: Koc = 12900

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be readily biodegradable, though the ten-day window may not be met. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 45200

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)

**Year:** 2004

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The estimated log Kow value of 7.07 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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**4.6.3 Toxicity to Soil Dwelling Organisms**

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**4.6.4 Toxicity to other Non-Mamm. Terrestrial Species**

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**4.7 Biological Effects Monitoring**

-

**4.8 Biotransformation and Kinetics**

-

**4.9 Additional Remarks**

-

## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** The results indicate that the test material was rapidly utilised for the biosynthesis of lipids in most tissues of the rat (heart, lungs, liver, intestine, kidney, brain and plasma). Most of the radioactive label was incorporated into the acyl moieties of both phospholipids and neutral lipids. The pattern of incorporation of radioactivity into the alkyl, alk-1-enyl and acyl moieties of the lipids suggested that oxidation and esterification of the resulting fatty acid to a wide variety of lipids are the predominant reactions. Acylation is observed mostly in the liver while alkylation to alkoxylipids occurred predominately in the heart. The presence of a large proportion of the dose (52%) in the lungs 1 hour after dosing and an increase in the proportion of radioactivity in acyl moieties at 24 hours suggests preferential deposition in the lungs followed by incorporation into lipids.

Radioactivity decreased most rapidly in the liver, kidneys and intestines.

**Test condition:** Groups of 5-9 male rats maintained on laboratory diet were injected intravenously (into the tail vein) with cis-9-[1-14C] octadecenol. The rats were killed at intervals of 1, 24, 48 and 96 hours after dosing. Lipids were isolated from major organs.

**Test substance:** cis-9-octadecenol

**Conclusion:** The test material was rapidly utilised for the biosynthesis of lipids in most tissues of the rat (heart, lungs, liver, intestine, kidney, brain and plasma).

This study was cited in the Cosmetic Ingredients Review, 1985.

**Reliability:** (2) valid with restrictions
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

06-NOV-2004 (11) (21)

**Result:** Oleyl alcohol at 200 mg/kg/day for 14 days did not cause any obvious ill effects. The distribution of major lipid classes in the heart, brain, kidneys, liver, testes, adipose tissue and blood was unaffected by treatment. Long chain alcohol did not accumulate in any of these tissues. In the small intestine only traces of the alcohol could be detected but wax esters were markedly elevated.

**Source:** Bandi et al, 1971

**Test condition:** A group of 30 Sprague-Dawley rats (average wt 200g) received 200 mg/kg/day oleyl alcohol (cis-9-octadecenyl alcohol) by stomach tube for 14 days. The control group consisted of 10 rats on basic diet.

Faeces were collected on days 12, 13 and 14. On day 15 pairs of rats which had received oleyl alchol were killed at half hourly intervals from 0 -7 hours after the last feeding. Blood was collected by heart puncture. Heart, brain, kidneys, liver, testes, adipose tissue and small intestine were collected,

weighed and stored at -10C in hexane for further processing.

Following extraction of lipids from the faecal, blood and tissue samples the distribution of lipid classes was analysed by TLC.

**Test substance:** oleyl alcohol (cis-9-octadecenyl alcohol)
**Reliability:** (2) valid with restrictions
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
10-NOV-2004 (8)

**Result:** A marked change was found in the lipid types in the liver but not in the brain. In the liver free and esterified long chain alcohols increased 3 fold.
**Test condition:** Groups of 4 male Wistar rats (body weight 150-200g) received basic diet supplemented with 160 mg cis octadecenol daily for 7 or 14 days.

At the end of the test period the animals were sacrificed and the liver and brian removed for analysis of tissue lipids.

Neutral lipids were analysed for free and esterified long chain alcohols and alkyl and alk-1-enyl glycerols. Total lipid phosphorus, alkyl acyl and alk-1-enyl acyl phosphoglycerides were determined in the phospholipid fraction.

**Test substance:** cis-9-octadecenol
**Reliability:** (2) valid with restrictions
10-NOV-2004 (11) (13)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22). This includes data reported for C14 (tetradecanol), C16 (1-hexadecanol), C18 (1-octadecanol) alcohols and data for C16-18 alcohols and C16-18 and C18 unsaturated alcohols. This data supports the statement that C18 unsaturated alcohols are expected to be of low acute oral toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (24) (28)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18, C18 (octadecanol) and C20 (eicosanol) alcohols in support of the statement that C18 unsaturated alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (24) (28)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category from C6-20). This includes data reported for tetradecanol, C16-18 alcohols and the C20 alcohol (1-eicosanol). This data supports the statement that C18 unsaturated alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (24) (28)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 23 hour(s)
**No. of Animals:** 6
**Result:** slightly irritating

**Method:** other: modification of Official French Method for Cosmetics and Toiletries

**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** All the samples tested as a 10% aqueous dispersion had scores between 0 and 0.5 with actual scores ranging from 0.04 to 0.41.

Undiluted samples were all considered slightly irritating with actual scores ranging from 1.33 to 1.75.

**Test condition:** Four samples of Oleyl alcohol from different manufacturers were tested. The composition of the samples was determined by GLC. Of the 4 samples tested one was less pure than the others.

The test method used was a modification of the French offical method for testing cosmetics and Toiletries, 1971 & 1973, this method (not described in the publication) involves a 23 hour occlusive exposure to intact and abraded rabbit skin. The degree of irritation is scored at 1 and 48 hours after patch removal. Modifications involved caging of the animals, fixing of the patches and a modification of the scoring. The official method classed a 0 response as non-irritant and 0-2 as slightly irritant. The modification considered 0-0.5 as non-irritant and 0.5-2 as slightly irritating. The score is presented as PII (as in the Draize test) with a maximum obtainable score of 8. 6 animals specified in Official method.

Each sample was tested undiluted and as a 10% aqueous dispersion using an emulsifier and preservative. Duplicate assays were carried out on two of the test samples.

**Conclusion:** All samples of oleyl alcohol tested were slightly irritating to rabbit skin when applied undiluted in a 23 hour occlusive exposure. They were not irritating when tested as 10% aqueous dispersions.

This study was cited in the Cosmetics Ingredient Review, 1985.

**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restirictions.

**Flag:** Critical study for SIDS endpoint

05-AUG-2005 (11) (14)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 9
**Result:** not irritating

**Method:** other: unspecified
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Report of unpublished data provided to CFTA, 1979.

In this 24 hour occlusive exposure to the skin of 9 rabbits an irritation score of 0.17 on a scale of 4 was reported indicating minimal skin irritation. No further details

available.
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
05-AUG-2005 (11)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Report of unpublished data provided to CFTA, 1979.

Undiluted oleyl alcohol was applied to rabbit skin on 4 consecutive days. On a scale of 4 the greatest average score was 2.33. This was considered to indicate mild primary irritation. No further details available.
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
05-AUG-2005 (11)

**Species:** rabbit
**Exposure:** no data
**Exposure Time:** 60 day(s)
**No. of Animals:** 3
**Vehicle:** other: applied undiluted as a 10% aqueous dispersion

**Method:** other: modification of Official French Method for Cosmetics and Toiletries
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The undiluted samples produced thickening and drying and cracking of the skin with eschars. Histological examination typically revealed hyperacanthosis and a flattened stratum corneum.

The 10% aqeuous dilutions were relatively well tolerated. Slight epidermal exfoliation was observed with 3 samples. Histological examination showed showed some vascular congestion of the dermis without inflammatory infiltration.

None of the test samples revealed evidence of hypersensitivity on challenge.
**Test condition:** Four samples of Oleyl alcohol from different manufacturers were tested. The composition of the samples was determined by GLC. Of the 4 samples tested one was less pure than the others.

The test method used was a modification of the French offical method for testing cosmetics and Toiletries, 1971 & 1973. The test material was applied daily for 8 weeks followed by a recovery period of 7 days. Excess test material was removed with gauze. After 8 weeks histological examination was made of 2 samples of skin from each rabbit. A challenge assay was incorporated to determine whether the reactions were of irritant or allergic origin. At least 3 animals specified in the guideline.

Each sample was tested undiluted and as a 10% aqueous dispersion using an emulsifier and preservative.

**Test substance:** Cas# 143-28-3 Oleyl alcohol
**Conclusion:** Repeated daily application of undiluted oleyl alcohol to the rabbit skin for 8 weeks resulted in drying and cracking of the skin with eschar. A 10% aqueous dilution was well tolerated. There was no evidence of an allergic response.
**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restirictions.
11-NOV-2004 (11) (14)

**Species:** human
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 48 hour(s)
**No. of Animals:** 50
**Result:** not irritating

**Method:** other: human patch test
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Oleyl alcohol was not irritant to human skin in this assay.
**Test condition:** 50 human volunteers (no atopics) received patches (15 mm diameter) with 0.05 g of the undiluted test material, these remained in place on the back for 48 hours. The patches were removed and the site swabbed with dry gauze to remove anyresidual test material. The test sites were scored 30 minutes after removal and up to 120 hours as necessary.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
10-NOV-2004 (20)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** no data
**No. of Animals:** 6
**Result:** not irritating

**Method:** other: modified Official French Method for Cosmetics
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** A maximum score for any of the samples was 7.17 observed at 1 hour after instillation. The scores diminished after this and all scores were 0 by day 3.
**Test condition:** Four samples of Oleyl alcohol from different manufacturers were tested. The composition of the samples was determined by GLC. Of the 4 samples tested one was less pure than the others.

The test method used was a modification of the French offical method for testing cosmetics and Toiletries, 1971 & 1973, this method (not described in the publication) involves

instillation of 0.1 ml or 100 mg undiluted material into the rabbit eye observations are made at 1, 2, 3, 4 and 7 days after instillation. Modifications to the test method involved using fluorescein, a retinograph and ophthalmoscope, a reading at 1 hour post instillation and use of an evaluation scale from 0-100 to evaluate the result. Scores under 10 with no evidence of corneal opacity were not considered significant.

Each sample was tested undiluted and as a 10% aqueous dispersion using an emulsifier and preservative. Duplicate assays were carried out on two of the test samples.

**Conclusion:** Oleyl alcohol when instilled either undiluted or as a 10% aqueous dispersion is not considered irritating to the rabbit eye.

This study is cited in the Cosmetics Ingredient Review, 1985.

**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restirictions.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (11) (14)

## 5.3 Sensitization

**Remark:** Oleyl alcohol (4 samples) was applied undiluted and as a 10% aqueous dispersion to the skin of rabbits for 60 days. At the end of this period a challenge application was made after a 7 day rest period. There was no evidence of allergic reaction.

Test more fully described under skin irritation.

**Test substance:** Oleyl alcohol C18 unsaturated alcohol.

**Reliability:** (2) valid with restrictions
Test procedure in accordance with national standard methods with acceptable restrictions.

05-DEC-2005 (14)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C18 unsaturated alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C16-18 and C18 unsaturated alchols, C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated

exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (23) (24) (28)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C18 unsaturated alcohols are available from studies of reliability 1 or 2 for C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, C16-18 and C18 unsaturated, hexadecanol and octadecanol [Ames].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
25-OCT-2005 (23) (24) (28)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (16) (23) (24) (28)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C18 unsaturated alcohols are not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol), C22 (docosanol) and the supporting substance C18 (octadecanol).

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (23) (24) (28)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C18 unsaturated alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

25-OCT-2005 (23) (24) (28)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: Human skin irritation

**Remark:** The purpose of this study was to introduce the chamber-scarification test designed for increased sensitivity for assessing the irritancy of materials. It is important to note that persons especially vulnerable to irritants were selected.

The materials were applied as a 25% solution in mineral oil. The skin is first scarified and the test material applied (0.1 ml) in a test chamber once daily for 3 days to groups of 5-10 volunteers. The skin was assessed 30 minutes after the end of the final exposure.

The degree of irritation was related to carbon chain length, the C10 and C12 alcohols giving a marked response while the C14 alcohol gave a moderate response, C16 slight and the oleyl alcohol gave a low response.

This work was presented at the 3rd conference on Cutaneous Toxicity, Washing DC, 1976 and published in the conference proceedings in Cutaneous Toxicity eds Drill & Lazar. This referred to by RTECS, 2004.

**Test substance:** oleyl alchol, hexadecyl alcohol, tetradecyl alcohol, dodecyl alcohol, decyl alcohol

**Reliability:** (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment.

11-NOV-2004 (12)

**Type:** other: Allergic reactions in man

**Remark:** Reports of patients reacting to formulations containing oleyl alcohol with a positive response when patch tested with oleyl alcohol.

**Test substance:** Oleyl alcohol

**Reliability:** (2) valid with restrictions

11-NOV-2004 (10) (10) (17) (25)

**Type:** other: Comparative skin irritation

**Result:** Oleyl alcohol was found to be severely irritating to the skin

of rabbits and guinea pigs, moderately irritating to rat skin but non-irritating to the skin of humans and minature swine.

**Test condition:** Animal studies: albino angora rabbits ave wt. 2.6 kg, Hartley guinea pigs 350-500g and Wistar rats 250-350g. Groups of 6 animals received 0.1g of undiluted test material to the shorn dorsal skin. The test material was allowed to remain in contact with the skin for 24 hours, uncovered. After 24 hours the skin reactions were scored and a further identical application made. At 48 hours the sites were scored again and then at 72 hours. The animals were then injected intravenously with Evans Blue dye and an hour later they were sacrificed and the dorsal skin removed. Minature swine were also tested receiving a 48 hour patch test with 0.05g of test material. The test site was evaluated as described above.

The intact skin was scored for redness (72 hours) while the excised skin was assessed for the dilating rate of blood vessels, oedema, bluing rate (indication of increased capillary permeability) and the bleeding rate. Scores for the various parameters were combined to give a so called primary irritation index (total score). Total score = dilating rate + swelling rate + bluing rate + bleeding rate + reddening rate. Scores <= 4 indicated mild irritation, 4-8 moderate irritation and >8 severe irritation.

Histopathological examination of the skin was also carried out.

Human studies: 50 human volunteers received patches with 0.05 g of the test material, these remained in place on the back for 48 hours and scored 30 minutes after removal and then at up to 120 hours as necessary.

**Test substance:** Oleyl alcohol (technical grade)

**Reliability:** (2) valid with restrictions
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

11-NOV-2004 (20)

**Type:** other: Allergic reaction in man

**Remark:** The authors report the results of patch testing with aliphatic alcohols in 1664 consecutive patients at a dermatological clinic. Patch testing with oleyl alcohol (30% in vaseline) resulted in 10 positive reactions and incidence of 0.6%. Of these 3 also reacted to stearyl alcohol suggesting cross sensitisation.

Cited in the Cosmetic Ingredient Review, 1985.

**Test substance:** Oleyl alcohol

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

11-NOV-2004 (11) (15)

**Type:** other: Human reaction to products containing oleyl alchol

**Remark:** The authors sumarise the results of patch tests in approx 600

subjects with various cosmetic products containing oleyl aclohol. None of the reactions were considered indicative of sensitisation
**Test substance:** Oleyl alcohol
**Reliability:** (4) not assignable
Secondary reference.

10-NOV-2004 (11)

**Type:** other: Allergic reaction in man

**Result:** Positive responses to oleyl alcohol were observed in 33 patients (9 male, 24 female) which is 23.2% of the total test population. A total of 34 subjects showed a positive reaction to fatty alcohols. Of these 11 patients had a positve reaction to their own topical preparations containing fatty alcohols and 18 had several positive reactions to other common ingredients of cosmetics or topical preparations.
**Test condition:** Between May 1992 and September 1995 146 patients, of both sexes aged 13-72 years with suspected cosmetic or medicament contact dermatitis, were patch tested with a series of 5 fatty alcohols. Fatty alcohols >99% pure were used for the patch testing. The materials were applied (30% in petrolatum) to the skin for 2 days using Finn chambers on Scanpor tape. Readings were made at 2, 3 and 7 days. 108 females and 38 males were tested.
**Test substance:** Oleyl alcohol 99% pure
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

06-AUG-2005 (26)

**Type:** other: Allergic reaction in man

**Result:** 13 patients patch tested with oleyl alcohol gave clear positive responses.
**Test condition:** 51 patients allergic to wool wax alcohols were tested with 13 wool wax derivatives using the ICDRG procedure. The test group of 24 females and 27 males were aged between 18 and 78. Oleyl alcohol was tested at 30% in vaseline.
**Test substance:** Oleyl alcohol
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

11-NOV-2004 (7)

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 629-96-9
**CAS No.** 629-96-9
**EINECS Name** icosan-1-ol
**EC No.** 211-119-4
**Molecular Formula** C20H42O

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
**Revision date:**
**Date of last Update:** **11-MAY-2006**

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**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

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03-AUG-2005

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**Remark:** Industry Consortium
23-AUG-2005

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**Remark:** Consortium Member
20-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
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20-DEC-2005

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**Name:** Sasol North America Inc.
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20-DEC-2005

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**Name:** Shell Chemical Company
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**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

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**Name:** Shell Chemicals Limited
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**Remark:** Consortium Member
20-DEC-2005

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**Name:** The Procter & Gamble Company
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**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company).

More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |

| | |
|---|---|
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original

documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Eicosanol
**Smiles Code:** OCCCCCCCCCCCCCCCCCCC
**Mol. Formula:** C20 H42 O1
**Mol. Weight:** 298.56

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-eicosanol, CAS 629-96-9 are >80% linear.

The substance comprises >=90% C20. Components of even chain length, in the range C18-22 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Eicosanol (6CI, 8CI, 9CI) (CA INDEX NAME)
Eicosanol (7CI)
1-Icosanol
Eicosan-1-ol
Icosan-1-ol
Icosanol
Some commercial products with the name Nacol
Some commercial products with the name Alfol
Arachic alcohol
Arachidic alcohol
Arachidyl alcohol
Eicosyl alcohol
n-1-Eicosanol
n-Eicosanol
NSC 120887

**Source:** Synonyms listed in various sources in the public domain,

including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-eicosanol.

Composition is described in section 1.1.1, General Substance Information

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >500 - 5 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus

import) for USA, for 2002. This is equivalent to >1 000 000 - 10 000 000 pounds.
21-DEC-2005 (7) (16) (22)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, the remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (24)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required

11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-eicosanol. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
03-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
03-AUG-2005

## 2.1 Melting Point

**Value:** = 66 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Documentation insufficient for assessment.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (14)

**Value:** = 64 - 68 degree C

**Method:** other: DAB 10 V.6.11.1
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint.
04-JAN-2005 (21)

## 2.2 Boiling Point

**Value:** = 309 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (13)

**Value:** = 372 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
04-JAN-2005 (20)

## 2.3 Density

**Type:** relative density
**Value:** = .8405 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** HSDB
**Reliability:** (2) valid with restrictions
Value obtained from secondary literature (HSDB). Cited

reference is a recognised source of chemical data
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (25)

**Type:** density
**Value:** = .8 - .804 g/cm³ at 4 degree C

**Method:** other: DIN 51757
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (15)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00000015 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Daubert and Danner 1989.
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data. This reference is considered as definitive for vapour pressure values.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005

**Value:** < 1 hPa at 20 degree C

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (15)

**Value:** = .00000016 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Result = 1.6 X 10-7 hPa
**Reliability:** (2) valid with restrictions

The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
19-SEP-2005 (1)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 7.75

**Method:** other (measured): Reverse-phase HPLC with mass spectrometry
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures. Test conditions: Column: 5 µm Ultrasphere-ODS 2.0 mm i.d. x 25 cm. Mobile Phase: Solution A: methanol:ethanol:water 70:15:15. Solution B: methanol:ethanol:water 95:5:0. 100% A for 1 min. Gradient to 100% B at 6.67% per min. 100% B for 30 min. Seven reference standards were used to correlate elution time with Kow. Dead time was measured using a non-retained substance (either acetone or acetonitrile).
**Reliability:** (2) valid with restrictions
Test is comparable to OECD guideline with some experimental differences and was not conducted to GLP.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (8)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .0027 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.0027 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
05-OCT-2005 (1)

**Solubility in:** Water

**Descr.:** not soluble

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
05-OCT-2005 (13)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 195 degree C

**Method:** other: DIN 51758
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
04-JAN-2005 (15)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 29.49879E-12 cm3/molecule.sec
Half-life: 13.1 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number, but the reported half-life represents a reasonably conservative estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
21-DEC-2005 (3)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
10-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 298.5
Data temperature 25 deg C
Log Kow 7.75
Water Solubility 0.0011 mg/l
Vapour pressure 0.000015 Pa
Melting point 66 deg C
half life in air 13.1 h
half life in water and soil 720 h
RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 1.61E-03% |
| Soil | 97.8% |
| Water | 1.96E-03% |
| Fish | 5.52E-03% |
| Sediment | 2.17% |

The Level III program has also been used, with the default model, using the same input parameters.The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 0.639 | 2.52E-05 | 2.41E-07 |
| % in water | 1.22 | 2.5 | 0.0111 |
| % in sediment | 47.5 | 97.5 | 0.433 |
| % in soil | 50.6 | 0.00199 | 99.6 |

The results reflect that the ultimate fate of 1-eicosanol is dependent on its route of release into the environment. 1-Eicosanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-eicosanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 3.3.2 Distribution

**Method:** other (calculation):various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The measured log Kow value of 7.75 was used in the TGD calculation methods.

**Result:** TGD hydrophobics method: Koc = 2390000

TGD Non-hydrophobics method: Koc = 112000
TGD Alcohols method: Koc = 3330
SRC PCKOCWIN method: Koc = 43800

Note: the TGD Alcohols method is valid up to log Kow = 5 and the Hydrophobics method is valid up to log Kow = 7.5. The results are presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** inherently biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be inherently biodegradable. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 31800

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log

Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The measured log Kow value of 7.75 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single

carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

**Result:** No chronic effects would be expected for this substance.
**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble

fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (9)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | Sprague-Dawley |
| **Sex:** | male/female |
| **No. of Animals:** | 20 |
| **Vehicle:** | other: 0.8% hydroxypropyl-methylcellulose gel |
| **Doses:** | 8250 and 10000 mg/kg |
| **Value:** | > 10000 mg/kg bw |
| **Method:** | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year:** | 1987 |
| **GLP:** | yes |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: All animals survived the 14 day observation period.<br><br>CLINICAL SIGNS: No clinical signs of toxicity. There was no adverse effect on food intake or bodyweight gain.<br><br>NECROPSY FINDINGS: Unremarkable.<br><br>POTENTIAL TARGET ORGANS: None identified.<br><br>SEX-SPECIFIC DIFFERENCES: None |
| **Source:** | Laboratory of Pharmacology and Toxicology 1987a<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Rat (Sprague-Dawley)<br>- Source: Lippische Versuchtierzucht, Hagemann GmbH, Extertal, Germany<br>- Age: 42-50 days<br>- Weight at study initiation: 156-168 g<br>- Group size: 5M+5F fasted<br>- Controls: no<br><br>ADMINISTRATION: Gavage<br>- Doses: 8250 and 10,000 mg/kg<br>- Doses per time period: single<br>- Volume administered or concentration: prepared using 0.8% hydroxypropyl-methylcellulose gel, dose concentration/volume not reported.<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Mortality, food and water consumption and weight gain were monitored during the observation period. All animals were subject to gross pathological examination. |
| **Test substance:** | Tradename Nacol 20 |
| **Conclusion:** | The rat oral LD50 for Nacol 20 is >10g/kg. At this dose level there was no evidence of toxicity in any of the parameters monitored. Reported in Iuclid 2000. |

**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
05-AUG-2005 (10) (12)

**Type:** LD50
**Species:** rat
**Strain:** no data
**Sex:** male
**No. of Animals:** 5
**Vehicle:** no data
**Doses:** no data
**Value:** > 64 ml/kg bw

**Method:** other: Smyth et al, 1962
**Year:** 1969
**GLP:** no data
**Test substance:** other TS: icosanol mixed isomers

**Result:** The rat oral LD50 for the mixed isomers of icosanol is > 64 ml/kg (>53760 mg/kg using the density of 0.84 g/cm3 reported in chapter 2.3).
**Source:** Smyth, 1969
**Test condition:** TEST ORGANISMS: Rat (Carworth-Wistar)
- Age: 5 weeks
- Group size: 5/group non-fasted
- Controls: no

ADMINISTRATION:
- Doses: not reported
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Mortality only. LD50 calculated using the methods of Weil (1952) and Thompson (1947).
**Reliability:** (2) valid with restrictions
Meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited. Rats were non-fasted. This study is also reported in Patty 2001.
11-MAY-2006 (17) (19)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** other: Carworth-Wistar
**Sex:** male/female
**No. of Animals:** 6
**Exposure time:** 8 hour(s)

**Method:** other: Smyth et al, 1962
**Year:** 1962
**GLP:** no data
**Test substance:** other TS: icosanol (mixed isomers)

**Result:** All rats survived this 8 hour static exposure to the concentrated vapours. LC50 > saturated vapour concentration.

**Source:** Smyth, 1969
**Test condition:** A group of 6 rats (sex unspecified) were exposed to concentrated vapours of the test substance for up to 8 hours using a static exposure technique.
**Reliability:** (4) not assignable
Screening test only, gives some indication of toxicity but exposure was static, methods described in an earlier publication Smyth et al. Am. In. Hyg. Assoc. J. 23:95-107, 1962.

This study is also reported in Patty 2001.
21-OCT-2004 (17) (19)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male
**No. of Animals:** 4
**Value:** > 20 ml/kg bw

**Method:** other: Smyth et al, 1962
**Year:** 1962
**GLP:** no data
**Test substance:** other TS: icosanol (mixed isomers)

**Result:** Results were not reported in detail. The LD50 was >20 ml/kg. (>16,800 mg/kg using the density of 0.84 g/cm3 reported in chapter 2.3). No further details available.
**Source:** Smyth, 1969
**Test substance:** TEST ORGANISMS: rabbit
- Source: no data
- Weight at study initiation: 2.5 -3.5 kg
- Group size: 4
- Controls: no

ADMINISTRATION: dermal
- Area covered: entire trunk
- Occlusion: Yes
- Vehicle: none
- Concentration in vehicle: undiluted

EXAMINATIONS: Clinical signs, 14 day observation period.
**Reliability:** (2) valid with restrictions
Meets generally accepted scientific principles, acceptable for assessment. Study considered valid although result reporting is limited.
11-MAY-2006 (19)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** other: rabbit, guineapig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: vaseline

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the

group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** Icosanol produced minimal reversible irritation to rabbit skin and was essentially non-irritating to human skin.
This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

**Reliability:** (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.

05-AUG-2005 (11)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of rabbit skin irritation test (OECD 404). The test material was reported as non-irritating.

Acute skin irritation/corrosion test (patch test) of Nacol 20 in the rabbit. Laboratory of Pharmacology & Toxicology, for Condea Chemie GmbH, 1986

**Test substance:** Tradename Nacol 20

**Reliability:** (4) not assignable
Secondary reference. (Study appears to be guideline and conducted at a contract laboratory but there are no experimental details to support this)

05-AUG-2005 (10)

**Species:** rabbit
**Concentration:** no data
**Exposure Time:** 24 hour(s)
**No. of Animals:** 5
**Vehicle:** no data
**Result:** slightly irritating

**Method:** other: Smyth et al, 1962
**Year:** 1962
**GLP:** no data
**Test substance:** other TS: Icosanol (mixed isomers)

**Result:** The skin irritation response was slight.
**Source:** Smyth, 1969
**Test condition:** This is a non-standard test. The test material is applied for a 24 hour uncovered exposure in a volume of 0.01 ml of either the undiluted material or dilutions in water or solvent. For this test the material was applied undiluted.

**Reliability:** (3) invalid
Non standard method not comparable to modern guidelines. This

result is also reported in Patty 2001.
21-OCT-2004 (17) (19)

## 5.2.2 Eye Irritation

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of rabbit eye irritation test (OECD 405). The test material was reported as slightly irritating.

Eye irritation study of Nacol 20 in the rabbit. Laboratory of Pharmacology & Toxicology, for Condea Chemie GmbH, 1986
**Test substance:** Tradename Nacol 20
**Reliability:** (4) not assignable
Secondary reference. (Study appears to be guideline and conducted at a contract laboratory but there are no supporting details)
05-AUG-2005 (10)

**Remark:** This eye irritation test is based on a protocol developed in 1946 (Smyth & Carpenter, 1946). This involves instillation of various volumes and concentrations into the eye and is not a valid test method. The result given was grade 1 which equates to at most a very small area of necrosis. This results is also reported in Patty 2001.
**Source:** Smyth, 1969
**Test substance:** other TS: Icosanol (mixed) isomers)
**Reliability:** (3) invalid
21-OCT-2004 (17) (19)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C22 alcohols are not expected to be skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (18) (23)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C20 (eicosanol) alcohols, from

studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (18) (23)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C20 (eicosanol) alcohol are available from studies of reliability 1 or 2 for hexadecanol, octadecanol [Ames] and docosanol [Ames, gene mutation, chromosome abberation].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (18) (23)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34), including data for hexadecanol, octadecanol and docosanol, are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol

[negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (18) (23)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C20 alcohol (eicosanol) is not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C16 (hexadecanol), C22 (docosanol) and the supporting substances C18 (octadecanol) and C24-34 alcohols.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (18) (23)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that eicosanol is not expected to be a developmental toxicant in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of

maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (18) (23)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(6) Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

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(9) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

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(17) Patty's Toxicology 2001 Bevan, C. Aliphatic alcohols (Monohydric alcohols) John Wiley & Sons - on line.

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(20) Syracuse Research Corporation (SRC) Online Database. Data obtained from a May 2002 online search.

(21) Technical data sheet for NACOL 20-96, Condea Chemie GmbH, 1993

(22) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(23) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 661-19-8 |
| **CAS No.** | 661-19-8 |
| **EINECS Name** | docosan-1-ol |
| **EC No.** | 211-546-6 |
| **Molecular Formula** | C22H46O |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **67** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

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03-AUG-2005

**Type:** lead organisation
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**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
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**Remark:** Consortium Member
20-DEC-2005

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20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
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20-DEC-2005

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**Name:** Mitsubishi Chemical Corporation
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**Remark:** Consortium Member
20-DEC-2005

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**Town:** 541-0051 Osaka
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**Remark:** Consortium Member
20-DEC-2005

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**Name:** Oleon N.V.
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20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
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**Town:** D-45764 Marl
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
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**Town:** 20138 Milano
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**Remark:** Consortium Member

20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
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**Town:** 77002 Houston, TX
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
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**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, Ohio
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**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** 1-Docosanol
**Smiles Code:** OCCCCCCCCCCCCCCCCCCCCC
**Mol. Formula:** C22 H46 O1
**Mol. Weight:** 326.61

21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** solid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as 1-docosanol, CAS 661-19-8 are 100% linear.

The substance comprises >95% C22. Components of even chain length are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

1-Docosanol (6CI, 8CI, 9CI) (CA INDEX NAME)
Lanette 22
n-Docosanol
NAA 422
Nacol 22-97
NSC 8407
Stenol 1822
Stenol 1822A
Tadenan
Some commercial products with the name Kalcol
Abreva
Behenic alcohol
Behenyl 80 Alcohol
Behenyl alcohol
Docosanol

Docosyl alcohol
IK 2
IK 2 (alcohol)

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in 1-docosanol.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >250 - 500 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >500 000 - 1 000 000 pounds.

21-DEC-2005 (7) (23) (28)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.
Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (30)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of 1-docosanol. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-AUG-2005

## 2.1 Melting Point

**Value:** = 72.5 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (20)

**Value:** = 69 - 73 degree C

**Method:** other: DAB 10 V.6.11.1
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (25)

**Value:** = 71 degree C

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
04-JAN-2005 (8)

## 2.2 Boiling Point

**Value:** = 401.1 degree C

**Method:** other: calculated (SRC MPBPVP v1.40)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The presence of branched components in the substance, within the limits described in section 1.1-1.4, is expected to raise the boiling point of those substances slightly, though it is not possible to predict values precisely.
Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP
**Reliability:** (2) valid with restrictions

The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** = 180 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test conducted at a pressure of 0.22 mm Hg.
**Reliability:** (2) valid with restrictions
Value obtained from a recognised source of physico-chemical data
11-OCT-2005 (20)

**Value:** = 180 degree C

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** by comparison with other measured values, it is considered likely that this result was obtained at reduced pressure.
**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
11-OCT-2005 (8)

## 2.3 Density

**Type:** density
**Value:** = .805 - .809 g/cm³ at 4 degree C

**Method:** other: DIN 51757
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Review of the original source (secondary literature) would not alter the reliability of this result.
**Flag:** Critical study for SIDS endpoint
04-JAN-2005 (25)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000000082 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** Result = 8.2 X 10-8 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** < 1 hPa at 20 degree C

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source (secondary literature) to reassign the reliability would not alter the overall conclusions concerning this endpoint. A source of higher reliability is available.
11-OCT-2005 (25)

## 2.5 Partition Coefficient

**log Pow:** = 7.75

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The presence of branched components is not expected to significantly affect the predicted value.
Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .0027 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.0027 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 195 degree C
**Type:** open cup

**Method:** other: DIN 51758
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Since it is based on company product data which cannot be validated further, review of the original source would not alter the reliability of these data.
04-JAN-2005 (21)

**Value:** ca. 227 degree C
**Type:** open cup

**Method:** other: ISO 2592
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Since it is based on company product data which cannot be validated further, review of the original source would not alter the reliability of these data.
04-JAN-2005 (25)

**2.8 Auto Flammability**

-

**2.9 Flammability**

-

**2.10 Explosive Properties**

-

**2.11 Oxidizing Properties**

-

**2.12 Dissociation Constant**

-

**2.13 Viscosity**

-

**2.14 Additional Remarks**

-

### 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 32.32488E-12 cm3/molecule.sec
Half-life: 11.9 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
09-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 326.6
Data temperature 25 deg C
Log Kow 7.75
Water Solubility 0.001 mg/l
Vapour pressure 0.00000815 Pa
Melting point 72.5 deg C

half life in air 11.9 h
half life in water and soil 720 h

RESULTS
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 1.05E-03% |
| Soil | 97.8% |
| Water | 1.96E-03% |
| Fish | 5.52E-03% |
| Sediment | 2.17% |

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 0.582 | 1.72E-05 | 1.71E-07 |
| % in water | 1.22 | 2.5 | 0.0111 |
| % in sediment | 47.5 | 97.5 | 0.434 |
| % in soil | 50.7 | 0.00149 | 99.6 |

The results reflect that the ultimate fate of 1-docosanol is dependent on its route of release into the environment. 1-Docosanol released to air would partially precipitate to soil and water. There is relatively little movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility. In water, the adsorption coefficient of 1-docosanol results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles,

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (4)

## 3.3.2 Distribution

**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

The estimated log Kow value of 7.75 was used in the TGD calculation methods.

**Result:**

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 2390000 |
| TGD Non-hydrophobics method: | Koc = 112000 |
| TGD Alcohols method: | Koc = 3330 |
| SRC PCKOCWIN method: | Koc = 149000 |

Note: the TGD Alcohols method is valid up to log Kow = 5. and

the Hydrophobics method is valid up to log Kow = 7.5. The results are presented for comparison only.
**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 12.4 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 37 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 8 day(s) = 16 %
10 day(s) = 23 %
14 day(s) = 29 %
22 day(s) = 33 %
28 day(s) = 37 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test material was exposed to activated sewage sludge micro-organisms at a concentration of 10 mg C/l with culture medium in sealed culture vessels in the dark at 21 C for 28 days.

The degradation of the test material was assessed by the determination of carbon dioxide produced. Control solutions with inoculum and the standard material, sodium benzoate, together with a toxicity control were used for validation purposes.
**Remark:** The following validity criteria were met:
(1) The IC/TC ratio of the test material suspension in the mineral medium at the start of the test was below 5%,
(2) the total CO2 evolution in the control vessels on day 28 was 37.85 mg/l (= 113.55 mg/3 l),
(3) degradation of reference substance reached pass level within 14 days,
(4) toxicity control (KALCOL 220-80 and sodium benzoate) degraded by 42% after 14 days, and
(5) results of parallel assay did not differ from each other by more than 20%.
**Result:** Kinetic of control substance:
8 days = 59%
10 days = 63%
14 days = 64%
22 days = 64%
28 days = 74%

The test material degraded <60% over the test period therefore it cannot be considered readily biodegradable.
**Test condition:** Concentration of inoculum: 30 mg suspended solids (ss)/l
Test volume: 3000 ml
Temperature: 21 C
pH: not reported
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (22)

## 3.6 BOD5, COD or BOD5/COD Ratio

**-**

## 3.7 Bioaccumulation

**BCF:** = 31800

**Method:** other: calculated (recalculated from Connell and Hawker, 1988)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

The estimated log Kow value of 7.75 was used in the calculation.
**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.
21-DEC-2005 (3)

## 3.8 Additional Remarks

**-**

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** semistatic
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LL50 :** > 1000
**Limit Test:** yes

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test material was prepared as a filtered Water Accommodated Fraction (WAF) by loading test medium with the respective amount of the test item. After stirring for 23 hours, the contents were left to settle for 1h. The mixture was then filtered through 0.2 um filters to give the 1000 mg/l loading rate filtered WAF.

**Result:** RESULTS: EXPOSED
LL50 > 1000 mg/l
Based on nominal loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Test condition:** TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Brow Well Fisheries, Hebden, Nr. Skipton, Yorkshire, UK
Weight: 0.89 g (mean)
Feeding: Commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 2 weeks prior to test
Feeding during test: None
Control group: 1 control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: None
Concentration of vehicle/solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Aerated vai narrow bore glass tubes
Alkalinity: Not reported
Hardness: approximately 100 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 1000 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 7
Test temperature: 14 C
Dissolved oxygen: 9.4 - 9.9 mgO2/l
pH mean: 7.9 - 8.1
TEST PARAMETER: Mortality
SAMPLING: Mortalities and adverse reactions were recorded at

3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-SEP-2005 (31)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: Survival, growth and reproduction rate
**Exposure period:** 21 day(s)

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Measured data of an acceptable quality are available for 21-day reproduction studies with Daphnia magna for the single

carbon chain length alcohols 1-octanol (111-87-5), 1-decanol (112-30-1), 1-dodecanol (112-53-8; supporting), 1-tetradecanol (112-72-1) and 1-pentadecanol (629-76-5). The studies are described in the relevant dossiers and in Annex X to the SIAR. The data were obtained generally in accordance with standard test guideline OECD 211. No measured data are available for mixtures of different carbon chain length alcohols.

The data suggest that for substances of chain length greater than C15, no chronic effects would be expected.

**Result:** No chronic effects would be expected for this substance.
**Reliability:** (2) valid with restrictions
Value estimated based on findings for similar substances (other Category members) in reliable studies.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (6)

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

**-**

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

**-**

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**-**

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble

fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (10)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 6
**Vehicle:** other: suspension in arachis oil
**Doses:** 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** OECD Guide-line 423
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period except for one female which showed a weight loss during the second observation week. This was considered unlikely to be a toxicological effect.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None considered of significance.

**Source:** Hempstock, 1997c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley-CD)
- Source: Charles River, Margate, Kent, UK
- Age: 8-12 weeks
- Weight at study initiation: males 217-246g, females 206-223g
- Group size: 3M initially followed when it appeared the males would survive by 3F, fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg
- Doses per time period: single dose
- Volume administered or concentration: 10 ml/kg at a concentration of 200 mg/ml in arachis oil.
- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to gross

pathological examination at the end of the observation period.
**Test substance:** Tradename Kalcol 220-80
**Conclusion:** The rat oral LD50 for Kalcol 220-80 is >2000 mgkg. There were no signs of intoxication and no remarkable findings on gross necropsy.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (12)

**Type:** LD50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: 0.8% hydroxypropyl-methylcellulose gel
**Doses:** 8250 and 10000 mg/kg
**Value:** > 10000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: No clinical signs of toxicity. There was no adverse effect on food intake or bodyweight gain.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None
**Source:** Laboratory of Pharmacology and Toxicology 1987b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Lippische Versuchtierzucht, Hagemann GmbH, Extertal, Germany
- Age: 42-50 days
- Weight at study initiation: 157-167 g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: 8250 and 10,000 mg/kg
- Doses per time period: single
- Volume administered or concentration: prepared using 0.8% hydroxypropyl-methylcellulose gel, dose concentration/volume not reported.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality, food and water consumption and weight gain were monitored during the observation period. All animals were subject to gross pathological examination.
**Test substance:** Tradename Nacol 22RD
**Conclusion:** The rat oral LD50 for Nacol 22 RD is >10g/kg. At this dose level there was no evidence of toxicity in any of the parameters monitored. This value is also reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (17) (19)

**Type:** LD50
**Species:** mouse
**Strain:** other: CF1
**Sex:** no data
**No. of Animals:** 10
**Vehicle:** other: olive oil
**Doses:** 1000 mg/kg
**Value:** > 1000 mg/kg bw

**Method:** other
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of an unpublished study from Henkel, 1977. A group of 10 mice (average wt. 25g) received a single dose of 1000 mg/kg in olive oil (heated) by stomach tube. None of the test animals died during the 8 day observation period. No further details available.
**Reliability:** (4) not assignable
Secondary reference.
06-AUG-2005 (9)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C16 (hexadecanol), C16-18, C18 (octadecanol) and C20 (eicosanol) alcohols in support of the statement that C22 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (26) (29)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for C16-18 alcohols and C20 (1-eicosanol) alcohols. This data supports the statement that C22 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (26) (29)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** water
**PDII:** 0
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The test material produced a primary irritation index of 0.0. No evidence of skin irritation was noted during the study other than very slight erythema at one test site at 1 hour after patch removal. All other scores were 0.
**Source:** Hempstock, 1997d
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.81 - 3.15 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 0.5 g of the solid test material was moistened with 0.5 ml distlled water and applied to the shorn dorsal surface of the skin.
- Area of exposure: 2.5 x 2.5 cm
- Occlusion: semi-occlusive

- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 72 hours
- Controls: None reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours post application

**Test substance:** Tradename Kalcol 220-80
**Conclusion:** Kalcol 220-80 is not a skin irritant when applied to rabbit skin undiluted in a 4 hour semi-occlusive exposure. Group mean 24+48+72 hours were 0.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (13)

**Remark:** Secondary report from Condea Chemie GmbH reported in Iuclid 2000. Acute skin/irritation/corrosion test (patch test) of Nacol 22 RD in the rabbit. Laboratory of Pharmacology and Toxicology, 1986

Study to OECD guideline 404, no further details available. Nacol 22 RD was not irritating to rabbit skin.
**Test substance:** Tradename Nacol 22RD
**Reliability:** (4) not assignable
Secondary reference.
06-AUG-2005 (17)

**Species:** other: rabbit, guineapig, hairless mouse, human volunteers
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: vaseline

**Method:** other
**Year:** 1977
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The most marked skin reactions were observed with rabbits, the degree of irritancy was related to carbon chain length. Minimal reactions were observed with the lower and higher chain alcohols with irritancy increasing from class 3 at C8, class 4 (C10 & 12)to a maximum class 5 at C14, then reducing to class 3 at C16 & 18. In most cases the human scores were less those of the rabbits and reached a peak of class 3 with the C10 aclohol. A similar pattern of response though much less marked (all scores classified as <=2) was observed with hairless mouse skin. The response in guineapigs followed no obvious pattern and all scores were classed as <=3.

The results for C8, C12, C14, C16 and C18 alcohols have been given descriptive ratings for rabbits and man in various Iuclid datasets on aliphatic alcohols and these ratings together with the actual gradings from this reference are

reported below.

1-hexanol: rabbit and man reaction class 1 (Kaestner 1977).
1-octanol: rabbit and man moderately irritating (Iuclid 2000 1-octanol); reaction class 3 for rabbits and 2 for man (Kaestner 1977).
1-decanol: rabbit reaction class 4, man class 3 (Kaestner 1977).
1-dodecanol: reaction class 4 for rabbits and 2 for man (Kaestner 1977).
Tetradecanol: rabbit highly irritating, man not irritating (Iuclid 2000 tetradecanol), rabbit reaction grade 5, man 1 (Kaestner 1977)
Hexadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
Octadecanol: rabbit reaction grade 3, man 1 (Kaestner 1977)
C20 and C22 alcohols: reaction grade 2 for rabbits and 1 for man.

**Source:** Kaestner, 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** In this comparative study C4-C22 fatty alchols were applied to the skin of rabbits, guineapigs, hairless mice and human volunteers in a 24 hour occluded exposure. The test sites were scored on a 5 class system as follows:

Class 1 (0-1 points) practically no skin irritation
Class 2 (2-5) causes marginal reactions in some animals of the group, which fade away rapidly
Class 3 (6-10) causes marginal or slight reactions, which fade away rapidly
Class 4 (11-20) causes clear reactions
Class 5 (>20) causes strong reactions

The results were represented in a bar chart comparing the reaction classes between species for each alcohol.

**Conclusion:** This comparative skin irritation study shows that the rabbit is the most sensitive test species. There is a relationship between carbon chain length with maximum response at C14 producing persistent strong skin reactions after a 24 hour occlusive exposure. Decanol and dodecanol produced clear skin reactions which did not regress rapidly. All other skin reactions (including those of human volunteers) were at most slight and rapidly reversible.

**Reliability:** (2) valid with restrictions
Comparative study well documented, meets generally accepted scientific principles, acceptable for assessment but not for classification.

06-AUG-2005 (17) (18)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4
**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0.53 (individual 24+48+72 hour mean scores 1, 0.3, 0.3).
- Conjunctivae (Chemosis): 0.1 (individual 24+48+72 hour mean scores 0.3, 0, 0)
- Overall irritation score: maximum group mean score (Draize 10.7).

DESCRIPTION OF LESIONS: Moderate conjunctival irritation was reported in all animals one hour after treatment with minimal to moderate conjunctival irritation at the 24 hour observation time. At 48 hours minimal conjunctival redness was observed in one animal only.

REVERSIBILITY: All scores were 0 at 72 hours.

OTHER EFFECTS: None reported.
**Source:** Hempstock, 1997e
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: 1 female, 2 males
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.80-2.90kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and was applied using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 62 mg)
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

**Test substance:** Tradename Kalcol 220-80
**Conclusion:** Kalcol is not classifiable as an eye irritant according to EU or GHS criteria.
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (11)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Secondary report of data from Laboratory of Pharmacology and Toxicology, 1986 cited in Iuclid 2000. Eye irritation study of Nacol 22 RD in the rabbit after single instillation into the conjunctival sac.

Study to OECD guideline 405, no further details available.
Nacol 22 RD was not irritating to the eye.
**Test substance:** Tradename Nacol 22RD
**Reliability:** (4) not assignable
Secondary reference.
06-AUG-2005 (17)

**Remark:** Summary report of an unpublished study from Henkel, 1977. 50 ul of a 1% dilution of behenyl alcohol in olive oil was instilled into the conjunctival sac of 5 rabbits. No further details available. Conjunctival irritation was scored at 2, 6, 24 and 48 hours postinstillation according to Draize, 1959. There were no corneal or iritic effects. Conjunctival irritation was observed at 2 and 6 hours postinstillation with mean conjunctival irritation scores of 18 and 10 respectively. There were no signs of conjunctival irritation at 24 and 48 hours. Based on these scores behenyl alcohol is not irritating to the eye.
**Test substance:** Behenyl alcohol
**Reliability:** (4) not assignable
Secondary reference.
19-OCT-2004 (9)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for, C16 (hexadecanol), C18 (octadecanol) which support the conclusion that C22 alcohols are not expected to be a skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (26) (29)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** rat **Sex:** male/female
**Strain:** other: CD
**Route of administration:** gavage
**Exposure period:** 26 weeks
**Frequency of treatment:** daily, 7 days/week
**Post exposure period:** No
**Doses:** 10, 100, 1000 mg/kg bw-day
**Control Group:** yes, concurrent vehicle
**NOAEL:** = 1000 mg/kg bw

**Method:** other: standard regulatory protocol
**Year:** 2000
**GLP:** yes

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 10, 100 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: One male at 100 mg/kg/day died on day 25, microscopic examination revealed changes consistent with aspiration of test material due to mis-dosing. There were no treatment related deaths.
- Clinical signs: None
- Body weight gain: Comparable in test and control groups.
- Food consumption: Comparable between test and control groups as was food efficiency.
- Ophthalmoscopic examination: No treatment related changes.
- Clinical chemistry: No treatment related changes.
- Haematology: No treatment related changes.
- Urinalysis: No treatment related changes.
- Organ weights: No treatment related changes.
- Gross pathology: No treatment related changes.
- Histopathology: No treatment related changes.
- Other: Concentrations of behenyl alcohol in the blood were measured on day 1 and in weeks 13 and 26. Maximum mean plasma conc. (Cmax) was observed 1 hour after dosing in all males and most females. 24 hours after dosing plasma concentrations were below the limit of quantification (<10ng/ml) at the 10 and 100 mg/kg dose levels while levels following administration of 1000 mg/kg/day remained quantifiable on each sampling day. Statistically significant differences in area under the curve (AUC24) were observed between males and females treated with 10 and 1000 mg/kg/day on day 1 and during week 13. The rate and extent of systemic exposure to rats as shown by AUC24 and Cmax on day 1 and in weeks 13 and 26 increased with increasing dose level. Increases were less than the proportionate dose increment and there was statistically significant evidence of non-proportionality on each sampling day.
STATISTICAL RESULTS: No statistically significant changes were observed in any of the parameters examined in the main study, the full results were therefore not presented in the publication. Statistical significance for monocytes, basophils, eosinophils and large unstained cell counts were not reported as these data were not normally distributed.

**Source:** Iglesias, 2002a

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 28-35 days
- Number of animals: 20M+20F per treated and control groups

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 26 weeks
- Type of exposure: Oral gavage, daily 7 days/week
- Post exposure period: No
- Vehicle: 1% aqueous Tween 80.
- Concentration in vehicle: 20% stock suspension for top dose diluted to give standard volume at lower doses
- Total volume applied: 5 ml/kg
- Doses: 0, 10, 100 and 1000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: 3 groups of 10M+10F treated and one group of 6M+6F controls for toxicokinetic studies after 26 weeks.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Twice daily
- Mortality: Twice daily
- Body weight: Weekly
- Food consumption: Weekly, food efficiencies calculated for first 14 weeks.
- Water consumption: Not recorded.
- Ophthalmoscopic examination: Prestudy and at weeks 12 and 25.
- Haematology: Samples obtained ex retro-orbital sinus from 10 rats/dose at weeks 12 and 25. Parameters monitored were Hb, PCV, RBC, WBC and differential count, platelet count, MCV, MCH, prothrombin time, abnormal cells, bone marrow smear.
- Biochemistry: Serum alkaline phosphatase, alanine and aspartate amino transferase, gamma-glutamyl transpeptidase, glucose, bilirubin, total cholesterol, urea, total triglyceride, total protein, Na, Cl, Ca, creatinine, inorganic phsohorus, electrophoretic protein.
- Urinalysis: From non-fasted water deprived rats. measurements were mde of pH, protein. Glucose, ketones, bilirubin, urobilinogen & blood (Multistiks), specific gravity, sediment analysis.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full
- Organ weights: Adrenals, brain, kidneys, liver, lungs (with main stem bronchi), ovaries, pituitary , prostate, spleen, testes, thymus, thyroid, uterus (with cervix).
- Microscopic: adrenals, brain, eyes & optic nerve, femur, heart, kidneys, liver, lungs, seminal vesicles, spinal cord, stomach, thyroid, uterus.

OTHER EXAMINATIONS: Blood taken from satellite groups (3M+3F) non-fasted on days 1, during weeks 13 and 26 at 0,.5, 1, 2, 4, 8 and 24 hours after dosing.

STATISTICAL METHODS: Organ & body weights Bartletts test followed by either a Behrens Fischer test (if Bartletts significant) or a Dunnetts test (if Bartletts not significant). Distribution of macroscopic and histopathological findings determined using a two-tailed Fischers Exact Test where appropriate. Haematological & biochemical parameters analysed using T-test.

**Test substance:** C22 alcohol - Docosanol (Behenyl alcohol)

**Conclusion:** NOAEL 1000 mg/kg/day. No adverse effects of statistical significance were seen in this well conducted study at any dose level. Cmax was reached in most instances at 1 hour post-dosing. Cmax and AUC increased with increasing dose level but the increase was not proportional.

**Reliability:** (2) valid with restrictions
Guideline study without detailed documentation (publication).

**Flag:** Critical study for SIDS endpoint

07-JAN-2006 (15)

**Type:** Sub-chronic

**Species:** dog **Sex:** male/female
**Strain:** Beagle
**Route of administration:** gavage
**Exposure period:** 26 weeks
**Frequency of treatment:** daily, 7 days/week
**Post exposure period:** no
**Doses:** 20, 200, 2000 mg/kg bw-day
**Control Group:** yes, concurrent vehicle
**NOAEL:** > 2000 mg/kg bw

**Method:** other: standard regulatory protocol
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: 2000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0. 20, 200 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No deaths among treated or control animals.
- Clinical signs: These were confined to observation of pale faeces in all dogs treated with 2000 mg/kg/day behenyl alcohol and 1 male and 3 females at 200 mg/kg/day. The incidence of this effect was variable and more pronounced in females. This was attributed to the presence in the gastrointestinal tract of unabsorbed test material. One control dog also had pale faeces on a single occasion.
- Body weight gain: No effects.
- Food/water consumption: No effects.
- Ophthalmoscopic examination: No treatment related changes.
- Clinical chemistry: No effects.
- Haematology: No effects.
- Urinalysis: No effects.
- Organ weights: No effects.
- Gross pathology: No adverse effects.
- Histopathology: No adverse effects.
- Other: Concentrations of behenyl alcohol in the blood were measured on day 1 and in weeks 13 and 26. Maximum mean plasma conc. (Cmax) was observed 2-16 hours after dosing independent of sex, dose level or sampling day. The rate and extent of systemic exposure to dogs as shown by AUC24 and Cmax on day 1 and in weeks 13 and 26 increased with increasing dose level. Increases were less than the proportionate dose increment and there was statistically significant evidence of non-proportionality on each sampling day.

STATISTICAL RESULTS: No statistically significant changes were observed in any of the parameters examined in the main study, the full results were therefore not presented in the publication. Statistical significance for reticulocytes, monocytes, basophils, eosinophils and large unstained cell counts was not reported as these data were not normally distributed.

**Source:** Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 19-23 weeks at start of study

- Number of animals: 4M+4F per dose level.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 26 weeks
- Type of exposure: Oral gavage
- Post exposure period: No
- Vehicle: 1% aqueous Tween 80
- Concentration in vehicle: 20% diluted to give standard volume.
- Total volume applied: 10 ml/kg
- Doses: 0, 20, 200 and 2000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Twice daily, full vetinary examination prestudy & weeks 11 & 24.
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly, food efficiency calculated weekly up to week 14.
- Water consumption: not recorded
- Ophthalmoscopic examination: Prestudy and weeks 12 & 25.
- Haematology: All dogs ex jugular vein, prestudy & weeks 12 & 25. Hb, PCV, RBC, WBC with differential count, platelets, MCV, MCH, prothrombin time, activated partial thromboplastin time, bone marrow samples taken from iliac crest at study end.
- Biochemistry: All dogs, prestudy & weeks 12 & 25. Serum alkaline phosphatase, alanine and aspartate amino transferase, gamma-glutamyl tracspeptidase, glucose, bilirubin, total cholesterol and trigyceride, total protein, Na, K, Cl and Ca. Inorganic phosphorus, electrophoretic protein, creatinine phosphokinase.
- Urinalysis: Fasted animals weeks 12 & 25. pH, protein. Glucose, ketones, bilirubin, urobilinogen & blood (Multistiks), specific gravity, ntirites & total reducing substances, sediment analysis.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full
- Organ weights: Adrenals, brain, kidneys, liver, lungs, ovaries, pituitary, prostate with urethra, spleen, testes, thymus, thyroid, uterus (with cervix).
- Microscopic: adrenals, brain, eyes & optic nerve, heart, kidneys, liver, lungs, spinal cord, stomach, thyroid, uterus.

OTHER EXAMINATIONS: Blood samples taken from all rats prestudy and during weeks 13 & 26 at 0.5, 1, 2, 4, 8 and 24 hours after dosing for toxicokinetic studies.

STATISTICAL METHODS: Organ & body weights Bartletts test followed by either a Behrens Fischer test (if Bartletts significant) or a Dunnets test (if Bartletts not significant). Distribution of macroscopic and histopathological findings determined using a two-tailed Fischers Exact Test where appropriate. Haematological & biochemical parameters and urinalysis was analysed using T-test.

**Test substance:** C22 alcohol - Docosanol [661-19-8] (Behenyl alcohol)

**Conclusion:** NOAEL 2000 mg/kg/day (dogs). No adverse effects were seen in this well conducted study at any dose level. Cmax was reached

at 2-16 hours post-dosing. Cmax and AUC increased with increasing dose level but the increase was not proportional.
**Reliability:** (2) valid with restrictions
Guideline study without detailed documentation (publication).
06-AUG-2005 (15)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Salmonella typhimurium reverse mutation assay
**System of testing:** S. typhimurium strains TA-1535, -1537, -1538, -98, -100
**Concentration:** 10, 100, 333, 667, and 1000 ug/plate
**Cytotoxic Concentration:** >1000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 471
**Year:** 2002
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested at concentrations up to 1000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: Assume >1000 ug/plate as dose levels were based on a cytotoxicity screen.
**Source:** Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent
**Test condition:** METHOD S. typhimurium reverse mutation assay. Carried out at a contract laboratory in Germany. This appears to be a standard OECD 471 assay although not all details are given in the publication.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA-1535, -1537, -1538, -98, -100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9

ADMINISTRATION:
- Dosing: 10, 100, 333, 667, and 1000 ug/plate based on a toxicity screen.
- Number of replicates: Two tests carried out each in triplicate
- Application: Plate incorporation assay, vehicle ethanol
- Positive and negative control groups and treatment: Negative: untreated and vehicle controls. Positive: Sodium azide , 4-nitro-O-phenylene diamine, 2-aminoanthracene.

CRITERIA FOR EVALUATING RESULTS:For a test to be considered positive there should be either a two fold (TA 100) or three fold (other strains) increase in reverse mutation rate or a dose related increase in revertants.
**Test substance:** C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]
**Conclusion:** Behenyl alcohol (C22) did not increase the reverse mutation

rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 1000 ug/plate.
**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (15)

**Type:** Mammalian cell gene mutation assay
**System of testing:** Chinese hamster V79 cells
**Concentration:** 2.0, 7.5, 15.0, and 20.0 ug/ml
**Cytotoxic Concentration:** >20 ug/ml
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 476
**Year:** 2002
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: no increase in mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Mean relative cell survival over the test concentrations ranged from 89.1 (20 ug/ml) to 93.8% (15 ug/ml).
- Without metabolic activation: Mean relative cell survival ranged from 96% (15 ug/ml) to 120.2 % (20 ug/ml).
**Source:** Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent
**Test condition:** METHOD: Appears to be OECD 476 although full details are not given in the publication. The tests were carried out at a contract laboratory in Germany.

SYSTEM OF TESTING:
- Species/cell type: Chinese hamster V79 cells.
- Deficiences/Proficiences: HGPRT deficient (selected by resistance to thioguanine)
- Metabolic activation system: The tests were carried in the presence and absence of S9 but the source of this metabolising fraction was not reported.

ADMINISTRATION:
- Dosing: 2.0, 7.5, 15.0, and 20.0 ug/ml
- Number of replicates: 2 independent assays were carried out.
- Application: Vehicle ethanol (final concentration of ethanol in the culture medium did not exceed 1%)
- Positive and negative control groups and treatment: Concurrent solvent and untreated controls. Positive controls were ethylmethanesulfonate and 7,12-dimethyl benzanthracene.
- Incubation time: 4 hours

CRITERIA FOR EVALUATING RESULTS: A reproducible concentration realated increase in mutation frequency.
**Test substance:** C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]

**Conclusion:** Behenyl alcohol (C22) did not increase the gene mutation rate in Chinese hamster V79 cells in the presence or absence of S9 at dose levels up to 20 ug/ml.
**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (15)

**Type:** Cytogenetic assay
**System of testing:** Chinese hamster V79 cells
**Concentration:** 0.6, 10.0 and 20.0 ug/ml
**Cytotoxic Concentration:** >20 ug/ml
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 473
**Year:** 2000
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No relevant increases in stuructural chromosome aberrations at any dose level.

PRECIPITATION CONCENTRATION: No reported.

MITOTIC INDEX: No increase in mitotic index (results not presented in the publication)

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No evidence of cytotoxicity at dose levels up to 20 ug/ml as evidenced by mitotic index or plating efficiency.

**Source:** Iglesias, 2002a
Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Chinese hamster V79 cells.
- Metabolic activation system: Rat liver S9 no other information given.
- No. of metaphases analyzed: 100 per replicate

ADMINISTRATION:
- Dosing: 0.6, 10 or 20 ug/ml for 18 hours; 20 ug/ml fo 7 or 24 hours.
- Number of replicates: Duplicates
- Application: Vehicle ethanol
- Positive and negative control groups and treatment:
- Incubation time: 7, 18 or 24 hours.
CRITERIA FOR EVALUATING RESULTS: A statistically significant dose related increase in structural chromosome aberrations or a significant postive response at one of the test points. Statistical analysis was only carried out for cells carrying aberrations-exclusive gaps. The X2 was included in the analysis.
**Test substance:** C22 alcohol CAS RN 661-19-8 [Behenyl alcohol]
**Conclusion:** Behenyl alcohol (C22) did not increase the incidence of chromosome aberrations in Chinese hamster V79 cells in the presence or absence of metabolising fraction at dose levels up to 20 ug/ml (highest dose level tested). There was no evidence

of cytotoxicity at this dose level.
**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (15)

**Type:** Ames test
**System of testing:** Salmonella typhimurium strains TA98 and TA100
**Concentration:** 0, 50, 150, 500, 1000 and 5000 ug/plate
**Cytotoxic Concentration:** >5000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: method K709.03 (Ames test)
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in either strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: >=500 ug/plate but this did not interfere with scoring of the plates.

CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.
**Source:** Thompson, 1997
Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98 and TA 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced

ADMINISTRATION:
- Dosing: 50, 150, 500, 1500 and 5000 ug/plate.
- Number of replicates: Single test performed in duplicate
- Application: Plate incorporation assay, vehicle tetrahydrofuran.
- Positive and negative control groups and treatment: Vehicle control- tetrahydrofuran. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5 or 1 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to vehicle controls.

**Test substance:** Tradename Kalcol 220-80
**Conclusion:** Kalcol 220-80 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions (only 2 strains and test not repeated).
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (27)

## 5.6 Genetic Toxicity 'in Vivo'

**Type:** Micronucleus assay
**Species:** mouse **Sex:** male/female
**Strain:** NMRI
**Route of admin.:** gavage
**Exposure period:** Single dose
**Doses:** 50, 150 500 mg/kg bw
**Result:** negative

**Method:** other: similar to OECD 474
**Year:** 2002
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: One male and one female mouse died either spontaneously or due to gavage error.

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: Not reported.

BODY WEIGHT CHANGES: Not reported.

FOOD AND WATER CONSUMPTION CHANGES: Not reported.

EFFECT ON PCE/NCE RATIO: No increase in the ratio.
No increase in the % of micronucleated erythrocytes.

GENOTOXIC EFFECTS: None for behenyl alcohol, the positive controls showed an appropriate response.

STATISTICAL RESULTS: No statistical significance.
**Source:** Iglesias, 2002a

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS:
- Age: At least 10 weeks
- Weight at study initiation: Not reported.
- No. of animals per dose: 6 males + 6 females

ADMINISTRATION:
- Vehicle: polyethylene glycol (PEG)
- Duration of test:
- Frequency of treatment: A single oral dose was administered.
- Sampling times and number of samples: 24, 48 or 72 hour harvest. At least one slide per sample (no other details

given). For each animal 1000 PCE's were scored for micronuclei.
- Control groups and treatment: Vehicle control (PEG), 30, 150 and 500 mg/kg Behenyl alcohol at a volume of 10 ml/kg bw. Positive control cyclophosphamide 40 mg/kg.

EXAMINATIONS:
- Clinical observations: Not reported
- Organs examined at necropsy: Not reported
- Criteria for evaluating results: A statistically significant dose-related increase in numbers of micronucleated polychromatic erythrocytes or a reproducible statistically significant positive response for at leats on of the test points. Statistical analysis used the Mann-Whitney test, significance at $p<0.05$.
- Criteria for selection of M.T.D.: 500 mg/kg/day was considered to be the maximum tolerated dose based on a previously conducted experiment however the criteria were reported.

**Test substance:** C22 alcohol [behenyl alcohol] CAS RN 661-19-8
**Conclusion:** Behenyl alcohol (C22) did not increase the % of micronucleated erythrocytes or the PCE:NCE ratio in mice at any time interval after treatment (24, 48 or 72 hours) at dose levels up to 500 mg/kg bw when compared to vehicle controls.
**Reliability:** (2) valid with restrictions
Comparable t guideline studye with acceptable restrictions. Similar to OECD 474 but full experimental details were not reported in the publication. In particular there were no details of toxicity to the mice although the top dose was reported as the MTD.
**Flag:** Critical study for SIDS endpoint
06-AUG-2005 (15)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Type:** other: fertility and reproductive toxicity
**Species:** rat
**Sex:** male/female
**Strain:** Sprague-Dawley
**Route of administration:** gavage
**Exposure Period:** Males for 71 days prior to mating until females were sacrificed. Females for 15 days prior to mating, during mating, and up to Day 17 of gestation.
**Frequency of treatment:** daily
**Premating Exposure Period**
**male:** 71 days
**female:** 15 days
**Duration of test:** 20th day of gestation
**No. of generation studies:** 1
**Doses:** 10, 100, 1000 mg/kg bw-day
**Control Group:** yes
**NOAEL Parental:** = 1000 mg/kg bw
**NOAEL F1 Offspring:** = 1000 mg/kg bw

**Method:** other: see text

**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: P1 and F1 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 10, 100 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1: None
- Body weight: Comparable between test and control groups.
- Food/water consumption: Comparable between test and control groups.
- Description, severity, time of onset and duration of clinical signs: One top dose male was sacrificed during week 6. There were no other remarkable clinical observations and the single death was not attributed to treatment.
- Fertility index: Not calculated
- Pregnancy rate: Number of pregnant animals 22, 22, 22 and 21 for controls, low, mid and high dose respectively.
- Precoital interval: Not reported.
- Duration of gestation: Comparable between treated and control groups.
- Gestation index: not calculated.
- Effects on sperm: No adverse effects.
- Hematological findings incidence and severity:
- Clinical biochemistry findings incidence and severity:
- Mortality: One top dose male was sacrificed during week 6.
- Gross pathology incidence and severity: Comparable in treated and control groups.
- Number of implantations: No significant difference between treated and controls. Implantations (mean) 17.2, 17.0, 18.1 and 18.0 for controls, low, mid and high dose respectively; Preimplantation loss 3.3, 8.3, 3.2, 5.8%; Postimplantation loss 4.7, 6.4, 6.3 and 5.8% for controls, low, mid and high dose respectively.
- Number of corpora lutea: No significant difference between treated and controls. Mean corpora lutea 17.8, 18.4, 18.7 and 18.9 for controls, low, mid and high dose respectively.
- Organ weight changes: No significant difference between treated and controls.
- Offspring toxicity F1 (gestation day 20):
- Litter size and weights: Comparable between treated and controls
- Sex and sex ratios: Comparable between treated and controls
- Viable young: Comparable between treated and controls. Viable young (mean) 16.4, 15.9, 17.0 and 16.9 for controls, low, mid and high dose respectively.
- Foetal examination: No macroscopic, internal or skeletal malformations or variations outside of historical control limits.

**Source:** Iglesias, 2002b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
Age/weight at study initiation: males 6-7 weeks old, 193-240g; females 10-11 weeks old, 208-262g
Number of animals: Groups of 22M+22F per dose level.

ADMINISTRATION / EXPOSURE

- Type of exposure: Gavage
- Duration of test/exposure: males 71 days premating until sacrifice of females (day gestation day 20), females 15 days premating until day 17 of gestation.
- Treatment: 0,10, 100 or 1000 mg/kg/day
- Control group and treatment: vehicle control
- Vehicle: 1% aqueous Tween 80
- Concentration in vehicle: 20% stock diluted to give standard dosing volume.
- Total volume applied: 5 ml/kg
- Doses: 0, 10, 100 and 1000 mg/kg/day

MATING PROCEDURES: males & females caged 1:1 during mating period, length of mating period unspecified.

STANDARDIZATION OF LITTERS: No

PARAMETERS ASSESSED DURING STUDY P:
- Clinical observations: Daily clinical signs, food & water consumption premating weekly (males), daily (females); gestation females (food & water) GD 0-2, 3, 6, 7-9, 10-13, 14-17 and 18-19. Body weights premating twice weekly F, then at GD 0, 3, 7, 10, 14, 18 and 20. Males twice weekly throughout exposure period. Complete macroscopic examination.
- Estrous cycle: Assessed by daily vaginal smears for 10 days prior to mating.
- Sperm examination: At the end of the study, a sperm count and measurement of sperm motility was carried out.
- Reproductive parameters: corpora lutea, pre & post impalntatons sites, early & late resorption sites, viable foetuses, position of foetuses in uterine horns

OFFSPRING: Examined at day 20 of gestation. Placental weights, viable foetuses, skeletal & visceral examination.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: males reproductive organs

STATISTICAL METHODS: one way analysis of variance and T-test on body weights, food & water consumption. Organ weights - Dunnetts or Behren's-Fischer's test. Nested analysis of variance and weighed t-test for fetal and palcental weights.

**Test substance:** C22 alcohol CAS RN 661-19-8 (behenyl alcohol)
**Conclusion:** NOAEL for reproductive effects 1000 mg/kg/day. There were no treatment related adverse effects on reproductive parameters at any dose level.
**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
**Flag:** Critical study for SIDS endpoint
11-MAY-2006 (16)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Species:** rat **Sex:** female
**Strain:** Sprague-Dawley
**Route of administration:** gavage
**Exposure period:** For 15 days prior to mating, during mating and up to Day 17 of gestation.

**Frequency of treatment:** daily
**Duration of test:** 20th day of gestation
**Doses:** 10, 100, 1000 mg/kg bw
**Control Group:** yes
**NOAEL Maternal Toxity:** = 1000 mg/kg bw
**NOAEL Teratogenicity:** = 1000 mg/kg bw

**Method:** other
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** All female rats survived to sacrifice and no maternal toxicity was observed. The were no differences between treated and control animals in any of the rerpoductive endpoints investigated (corpora lutea, pre & post implantation sites, early & late resorption sites). The litter size, foetal weight and sex ratio observed in treated groups was comparable to the control group. There were no unusual macroscopic findings among foetuses. Microscopic examination did not show any increased incidence of anomalies in skeletal or soft tissues. See above chapter 5.8.1 for further details.
**Source:** Iglesias, 2002b
Hayes Consultancy Service Bromley, Kent
**Test condition:** This study was part of a reproductive/development study in rats. The study is fully reported in Chapter 5.8.1 Fertility. Female rats, 5-6 weeks of age received 0, 10, 100 or 1000 mg/kg bw of behenyl alcohol by gavage as an aqueous suspension with a constant dosing volume of 5 ml/kg. The females were mated to treated males. Females received the the test material for 15 days prior to mating, throughout mating and up to Day 17 of gestation. Reproductive endpoints were evaluated at day 20 of gestation were corpora lutea, pre & post implantation sites, early & late resorption sites, viable foetuses, position of foetuses in uterine horns. In addition, foetuses were weighed and examined for abnormalities. The neck, thoracic and abdominal cavities were examined and a microscopic skeletal examination was performed. Statistical analyses were performed on all endpoints.
**Test substance:** C22 alcohol CAS RN 661-19-8
**Conclusion:** 1000 mg/kg/day is the NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rats receiving behenyl alcohol by gavage for 15 days premating, during mating and up until gestation day 17. This is based on the absence of adverse effects in any of the parental, reproductive or foetal parameters examined.
**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).
**Flag:** Critical study for SIDS endpoint
11-MAY-2006 (16)

**Species:** rabbit **Sex:** female
**Strain:** New Zealand white
**Route of administration:** gavage
**Exposure period:** days 6-19 of gestation
**Frequency of treatment:** daily
**Duration of test:** 28 days
**Doses:** 125, 500, 2000 mg/kg bw
**Control Group:** yes

**NOAEL Maternal Toxity:** > 2000 mg/kg bw
**NOAEL Teratogenicity:** > 2000 mg/kg bw

**Method:** other: ICH Harmonized Tripartite Guideline for Detection of Toxicity to Reproduction for Medicinal Products
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: 2000 mg/kg/day for maternal and foetal effects.

ACTUAL DOSE RECEIVED: 0, 125, 500, 2000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 20 (controls and top dose), 19 (125 and 500 mg/kg/day)
- Number aborting/total litter loss: A total of 3 females, one each in the control group and the 125 and 500 mg/kg groups were observed to have a total litter loss, the uterus of each female revealed early resorptions.
- Number of resorptions: Comparable to controls. Total resorptions (mean) 1.3, 1.3, 1.7 and 1.6; Early resorptions 0.4, 0.3, 0.4 and 0.7; Late resorptions 1.0, 1.1, 1.2, 0.9 for controls, low, mid and high dose groups respectively.
- Number of implantations: Comparable to controls.
- Pre and post implantation loss: Comparable to controls. Implantation loss pre 10.4, 14.2, 13.9 and 13.5%; Post 12.1, 12.0, 15.2, 14.7 for controls, low, mid and high dose groups respectively.
- Number of corpora lutea: Comparable to controls. Mean Corpora lutea 12.8, 12.9, 12.6 and 12.2 for controls, low, mid and high dose groups respectively.
- Duration of Pregnancy: Comparable to controls.
- Body weight, food/water consumption: Comparable to controls.
- Description, severity, time of onset and duration of clinical signs: The only clinical observations were of pale faeces in most females at the top dose level attributed to the presence of unabsorbed behenyl alcohol in the gastro-intestinal tract.

FETAL DATA:
- Litter size and weights, Number viable, Sex ratio: Comparable to controls. Viable young total 10.1, 9.8, 9.3 and 9.0 for controls, low, mid and high dose groups respectively.
- Anomalies: Macroscopic, visceral and skeletal examination of the foetuses revealed no variations which were outside the historical control incidence. Actual data were not reported.

**Source:** Iglesias, 2002b

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
Groups of 22 female New Zealand White rabbits aged ca 20-28 weeks at initiation (weight 3.29 - 4.98 kg)

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage
- Duration of test/exposure: Days 6-19 of gestation
- Control group and treatment: vehicle control
- Vehicle: 1% aqueous Tween 80

- Concentration in vehicle: 20%
- Total volume applied: 10 ml/kg for top dose and controls, 0.625 and 2,5 ml/kg for the 125 and 500 mg/kg dose level respectively.
- Doses: 0 125, 500 and 2000 mg/kg behenyl alchol.

MATING PROCEDURES: Mated with proven fertile males then injected with luteinizing hormone to ensure ovulation.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain and water consumption: Daily
- Food consumption: Days 1-5, 6-12, 13-19, 20-23 and 24-28 inclusive.
- Clinical observations: Daily
- Examination of uterine content: On gestation day 29, pre and post-implantation sites, early & late resrption sites, viable foetuses and distribution in uterine horn. The ovaries were examined for numbers of coprora lutea.
- Examination of fetuses: Foetal and placental weights were recorded. All foetuses were examined macroscopically for abnormalities. All foetuses were subjected to visceral examination microscopically and stained for skeletal examination. The heads of 1/3 of the foetuses were also sectioned and examined.

STATISTICAL METHODS: STATISTICAL METHODS: one way analysis of variance and T-test on body weights, food & water consumption. Organ weights - Dunnetts or Behren's-Fischer's test. Nested analysis of variance and weighed t-test for foetal and placental weights.

**Test substance:** C22 alcohol CAS RN 661-19-8

**Conclusion:** The NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rabbis, receiving C22 alcohol by gavage on gestation days 6-19, is 2000 mg/kg/day (top dose level). This is based on lack of statistically significant effects in the maternal, reproductive and foetal parameters evaluated at any dose level.

**Reliability:** (2) valid with restrictions
Comparable to guideline study without detailed documentation (publication).

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (16)

## 5.8.3 Toxicity to Reproduction, Other Studies

**Type:** other: Effects on the rat prostate
**In Vitro/in vivo:** In vivo
**Species:** rat
**Strain:** Wistar **Sex:** male
**Route of administration:** gavage
**Exposure period:** 28 days
**Frequency of treatment:** daily
**Duration of test:** 29 days
**Doses:** 1, 10, 100 mg/kg
**Control Group:** yes, concurrent vehicle

**Method:** other
**Year:** 1979
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Docosanol administered by gavage to rats aged 6-7 months for 28 days did not affect bodyweight or the weights of any of the organs weighed other than a statistically significant increase in weight of the seminal vesicles at the lower dose levels (1 and 10 mg/kg/day). There were no histological differences in the accessory sexual organs.

The concentration of radioactive zinc was decreased at 1 and 10 mg/kg in the dorsolateral prostate and increased in muscle at 10 and 100 mg/kg. At 100 mg/kg RNA concentration of the ventral prostate was increased but RNA content remained unchanged. The DNA content and concentration was also unchanged, the quotient between the conentrations of RNA and DNA was increased at 100 mg/kg. Protein concentration was unchanged. Plasma LH was increased at 100 mg/kg while FSH and prolactin were unaffected.

In the older rats the weight of the dorsal prostate was decreased to 85% of the weight of controls by 1 mg/kg and the weight of the seminal vesicles increase to 125% at 10 mg/kg. Spleen weight was decreased to 80% by 1 and 100 mg/kg docosanol. The quotient between RNA and DNA concentration was increased (130%) in the ventral prostate at 100 mg/kg. There were no histopathological changes in the organs examined. Plasma testosterone was reduced at 100 mg/kg and prolactin cncentration at 1 or 10 mg/kg.

Orchidectomy resulted in a significant increase in weight of prostate, seminal vesicles and adrenals at 100 mg/kg docosanol but not at lower dose levels. The concentration of radioactive zinc was reduced in the dorsolateral prostate at 10 or 100 mg/kg.

Docosanol did not increase the prostrate weight in rats which had been both orchidectomised and adrenalectomised suggesting a role for the adrenals in stimulating the prostrate.

Studies in young rats suggested a thymolytic effec as 100 mg/kg docosanol reduced the weith of both thymus and splenn in intact animals.

**Source:** Muenzing, 1979

**Test condition:** This study was carried out to investigate the mode of action of docosanol, the active principle of Tadenan, a drug used in the treatment of benign prostatic hyperplasia.

As part of this study groups of 7 or 8 rats aged 6-7 months were dosed daily for 28 days with 1, 10 or 100 mg/kg docosanol or with the vehicle at a dosing volume of 1 ml/kg. The vehicle was a solution of 4% isopropyl myristate and 4% benyl benzoate in peanut oil. On day 28 the animals received an ip injection of radiolabelled zinc, the rats being weighed and sacrificed by decapitation 24 hours later.

Blood was taken for measurement of plasma FSSH, LH and prolactin. The ventral and dorsolateral prostates, coagulating glands, seminal vesicles, adrenal glands, testes and spleen were weighed. The accessory sexual organs were examined histopathologically. The radioactivity of the ventral and

dorsal prostates, coagulating glands and rectus abdominus muscle was determined. DNA , RNA and protein concentrations were analysed in samples from the ventral prostate.

Groups of 8 older male rats aged 15-18 months were subject to the same dosage regime and examinations as above with the addition of determinations of plasma testosterone, dihydrotestosterone and androstenedione.

Similar investigations were made in rats aged 15-18 months) which had been, orchidectomised or orchidectomised and adrenalectomised. Dosing started 14 days after surgery and continued for 14 days.

A final experiment comprised groups of 10 young male rats aged 21-24 days half of which were adrenalectomised and which received daily doses of icosanol for 3 days.

**Conclusion:** Docosanol had no effect on the weight or histology of the prostate in intact rats but increased the RNA/DNA quotient in the ventral prostate. Plasma LH and testosterone were reduced. In orchidectomised rats docosanol increased the prostate and adrenal weight but there was no increase in orchidectomised adn adrenalectomised rats, a weight reduction being observed. Also docosanol had a thymolytic effect in intact rats but not in adrenalectomised rats where the thymus weight was increased. These results suggest a stimulation of adrenal steroid secretion but this may not be the only effect of docosanol.

This study was reported in the Hazardous Substances Data Bank, 2004

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

21-OCT-2004 (14) (24)

## 5.9 Specific Investigations

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## 5.10 Exposure Experience

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## 5.11 Additional Remarks

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(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(6) Annex X (2005). Chronic Toxicity of Long Chain Alcohols to Daphnia magna; Annex X to the Long Chain Aliphatic Alcohols SIAR.

(7) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(8) Chemical Rubber Company Atlas of Spectral Data and Physical Constants for Organic Compounds. CRC Press, Cleveland,Ohio, second edition, 1975

(9) Cosmetic Ingredient Review (CIR) 1988 Final report on the safety assessment of cetearyl alcohol, cetyl alcohol, isostearyl alcohol, myristyl alcohol and behenyl alcohol. J. Am. Coll. Tox. 7(3):359-413

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(11) Hempstock, 1997e Kalcol 220-80: Acute eye irritation test in the rabbit SPL Project Number: 140/722.

(12) Hempstock, C 1997c Kalcol 220-80: Acute oral toxicity study in the rat - acute toxic class method. SPL Project Number: 140/270

(13) Hempstock, C. 1997d Kalcol 220-80: Acute dermal irritation test in the rabbit. SPL Project Number: 140/721.

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Reproduction studies in rats and rabbits. Regulatory Tox. and Pharm. 36, 80-85.

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(22) Mead, C. 2000. Kolcol 220-80: Assessment of ready biodegradability; CO2 evolution test. Safepharm Laboratories, SPL Project Number 140/1002.

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 63393-82-8 |
| **CAS No.** | 63393-82-8 |
| **EINECS Name** | Alcohols, C12-15 |
| **EC No.** | 264-118-6 |
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **28-DEC-2005** |
| **Number of Pages:** | **42** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

03-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

### 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
03-AUG-2005

### 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C12-15 alcohols, CAS 63393-82-8 are >40% linear.

The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C10-C17 are present.

Commercial products marketed under this CAS number fall into two types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A and Type B.

Type A products are >80% linear. The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C10-C17 are present.

Type B products are 40-50% linear. The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C11-C16 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C12-15 (CA INDEX NAME)
Alc., C12-15
Alchem 125
Alcs., C12-15
C12-15 alcohols
Dobanol 25
Dobanol 25L
Neodol 25

Neodol 25E
Oxocol 1215

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C12-15 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (4) (7) (14)

### 1.6.1 Labelling

**Remark:** Not required

11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required

11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required

11-AUG-2003

### 1.7 Use Pattern

**-**

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-15 alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

11-AUG-2003

## 2.1 Melting Point

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
**Reliability:** (2) valid with restrictions
11-OCT-2005 (1)

## 2.2 Boiling Point

**Value:**

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (13)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0005 - .00053 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.00050 hPa
Type B: 0.00053 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** < .1 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
Value obtained from secondary literature. Original reference not stated.
11-OCT-2005 (10)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 5.3 - 6.4 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The substance has a range of components, as described in section 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value. Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water

**Value:** = .63 - .67 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.63 mg/l at a loading rate of 1000 mg/l
Type B: 0.67 mg/l at a loading rate of 1000 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
09-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4.

However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure).

Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint
11-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**
TGD Hydrophobics method: Koc = 27600 - 203000
TGD Non-hydrophobics method: Koc = 6420 - 23100
TGD Alcohols method: Koc = 390 - 1020
SRC PCKOCWIN method: Koc = 330 - 2050

These ranges of Koc values apply to both compositional Types A and B.

**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 2 mg/l related to Test substance
5 mg/l related to Test substance
**Contact time:** 30 day(s)
**Degradation:** = 100 % after 30 day(s)
**Result:** readily biodegradable

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

**Year:** 1985
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier (nonylphenol ethoxylated propoxylated, NP+9.5 EO+5PO) at a 1:1 ratio. Degradation rate of test substance was corrected by oxygen uptake of blank inoculum and emulsifier control. Oxygen concentrations were determined by iodometric titration according to Winkler. The values reported in the results section are for the 2 mg/l concentration. The 5 mg/l concentration test substance had insufficient residual dissolved oxygen content.

The following results were given, 5 day 50%; 15 day >60%; 30 day >60%.

The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound (Sodium benzoate) reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.

**Result:** 5 days = 70%
15 days = 100%
30 days = 100%
The substance degraded >60% in the 10 day window. The reference substance, Sodium benzoate degraded by 95% after 30 days.

**Test condition:** Inoculum concentration: 1 ml/l (about 10E3 - 10E5 cells/ml)
Test volume: 292.7-296.4 ml
Temperature: 20 C
pH: not reported

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (8)

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to all compositional Types.

The presence of branched components in the substance, within

the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 4500 - 42600

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Result:** Type A: BCF estimated as 7200 - 42600
Type B: BCF estimated as 4500 - 42600.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 2.4 - 2.6 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 2.4 mg/l
Type B: 2.6 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .21 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A and type B: 0.21 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - .3

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

For both compositional Types A and B, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The values obtained by prediction are:
Types A and B: both 0.1 - 0.3 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (2)

**4.4 Toxicity to Microorganisms e.g. Bacteria**

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**4.5 Chronic Toxicity to Aquatic Organisms**

**4.5.1 Chronic Toxicity to Fish**

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**4.5.2 Chronic Toxicity to Aquatic Invertebrates**

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**TERRESTRIAL ORGANISMS**

**4.6.1 Toxicity to Sediment Dwelling Organisms**

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**4.6.2 Toxicity to Terrestrial Plants**

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**4.6.3 Toxicity to Soil Dwelling Organisms**

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**4.6.4 Toxicity to other Non-Mamm. Terrestrial Species**

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**4.7 Biological Effects Monitoring**

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**4.8 Biotransformation and Kinetics**

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also

molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (5)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

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## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | Sprague-Dawley |
| **Sex:** | male/female |
| **No. of Animals:** | 16 |
| **Vehicle:** | other: undiluted |
| **Doses:** | 15.4, 23.1, 34.6 and 51.9 g/kg |
| **Value:** | = 26400 mg/kg bw |
| **Method:** | other: standard contract laboratory procedure |
| **Year:** | 1964 |
| **GLP:** | no |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY:<br>- Time of death: 3-8 days after dosing<br>- Number of deaths at each dose: 1/4, 2/4, 2/4, 4/4<br><br>CLINICAL SIGNS: At all dose levels diarrhoea and emaciation were reported with an onset 5-24 hours after administration and persisting for 2-7 days.<br><br>NECROPSY FINDINGS: Not carried out.<br><br>POTENTIAL TARGET ORGANS: None identified.<br><br>SEX-SPECIFIC DIFFERENCES: Male and female data were combined. |
| **Source:** | Shell 1964.<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Rat (SD)<br>- Source: no data<br>- Weight at study initiation: mean 110 grams<br>- Group size: 2M+2F fasted<br><br>ADMINISTRATION: gavage<br>- Doses: 15.4, 23.1, 34.6 and 51.9 g/kg<br>- Doses per time period: single<br>- Volume administered or concentration: undiluted<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Clinical observations and mortalities were recorded during the observation period. No necropsy.<br><br>STATISTICAL METHODS: The LC50 was calculated using the methods of Weil (1952) and Thompson & Williams (1947 and 1952) |
| **Test substance:** | Tradename Neodol 25 C12-15 alcohols Type A |
| **Conclusion:** | The rat oral LD50 for Neodol 25 was 26.4 g/kg. Signs of intoxiciation were diarrhoea and emaciation. No target organ was identified. |

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment, small group sizes.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (9)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C10 (1-decanol), C12 (1-dodecanol), C12-16, C14 (tetradecanol) and C16 (hexadecanol) alcohols in support of the statement that C12-15 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (11) (15)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 2
**Vehicle:** other: undiluted
**Doses:** 3, 4.5, 6.8 and 10.2 g/kg
**Value:** > 10200 mg/kg bw

**Method:** other: Contract laboratory screening protocol
**Year:** 1964
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 14 day observation period.

APPLICATION SITE: Moderate oedema and mild subdermal haemorrhaging was observed at all dose levels. Time of onset was 24 hours following administration with a duraton of 2-5 days.

CLINICAL SIGNS: Emaciation and inactivity observed at all dose levels.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported.

**Source:** Shell 1964
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand white)
- Source: Not reported
- Age: young adults
- Weight at study initiation: average weight 2.5 kg
- Group size: 1M+1F
- Controls: no

ADMINISTRATION: 24 hour occlusive application to intact skin.
- Area covered: 10% of body surface clipped for application.
- Occlusion: Plastic film.
- Doses: 3, 4.5, 6.8 and 10.2 g/kg
- Removal of test substance: Not reported.

EXAMINATIONS: Mortality, clinical signs and skin irritation were observed throughout the 14 day observation period.

**Test substance:** Tradename Neodol 25 C12-15 alcohols Type A

**Conclusion:** The rabbit dermal LD50 (24 hour occluded) for Neodol 25 was > 10.2 g/kg. All rabbits survived the exposure and clinical signs were emaciation and inactivity. Skin irritaiton was observed at the application site.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment, small group size.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (9)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 4
**Vehicle:** other: undiluted
**PDII:** 2.7
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1964
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE: The scores were presented as combined erythema and oedema scores for individual rabbits for intact and abraded skin. It is not possible to present the data in an EU/GHS format. The test material is described as mildly irritating with a Primary Irritation Rating of 2.7 (max. 8)

REVERSIBILITY: Skin irritation was still present at 72 hours.

OTHER EFFECTS: Not reported.

**Source:** Shell, 1964
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: Albino
- Sex: Not reported.
- Source: Not reported.
- Age: Not reported.
- Weight at study initiation: Not reported.
- Number of animals: 4
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour occlusive application to intact and abraded skin.
- Preparation of test substance: Undiluted
- Area of exposure: 2.5 cm square.
- Occlusion: Occlusive
- Vehicle: None
- Total volume applied: 0.5 ml
- Postexposure period: 72 hours
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours after exposure.

**Test substance:** Tradename Neodol 25 C12-15 alcohols Type A

**Conclusion:** Neodol 25 is considered mildly irritating according to the Draize scoring system with a PII of 2.7, following a 24 hour occlusive application to rabbit skin. It is considered that this degree of irritation in a Driaze test would not trigger classification according to EU criteria and would at most suggest a GHS classification as a mild irritant.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (9)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1964

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE The scores were reported as prescribed by the FDA 1959. Although individual animal data are provided only the converted scores are reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each time point was as follows:

1 hour: 11.6; 24 hours: 5.2
All other time points up to 7 days scored 0 for all parameters.

DESCRIPTION OF LESIONS:
- Cornea: There were no corneal effects, all scores were 0.
- Iris: 4 eyes scored 1 for iritis at 1 hour after instillation the remaining eye scored 2. At 24 hours 2 eyes scored 1 at all other time points there was no iritis, all scores 0.
- Conjunctivae (Redness and chemosis): Redness and/or chemosis was observed in all eyes at 1 hour and in 4/5 eyes at 24 hours post instillation. Scores at all other time points were 0.

REVERSIBILITY: The slight effects on the iris and conjunctivae at 1 and 24 hours post instillation were completely reversed by 48 hours. All eyes continued normal until the endof the observation period.

OTHER EFFECTS: None reported.

**Source:** Shell, 1964
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported.
- Source: Not reported.
- Age: Young adults
- Weight at study initiation: Not reported.
- Number of animals: 5
- Controls: The untreated eye served as a control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: undiluted
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: Not reported.
- Scoring system: Draize
- Observation period: at 1, 24, 48, 72 and 96 hours and then at 7 days.
- Tool used to assess score: Not reported.

**Test substance:** Tradename Neodol 25 C12-15 alcohols Type A

**Conclusion:** Neodol 25 applied undiluted to the rabbit eye is not classifiable as an eye irritant by either EU or GHS criteria. Although scores are not presented in the EU format it is obvious that the degree of irritation seen would not trigger classification.

**Reliability:** (2) valid with restrictions

Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (9)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A), C14 (tetradecanol) and C16 (hexadecanol) alcohols which support the conclusion that C12-15 alcohols are not expected to be skin sensitisers
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
05-DEC-2005 (11) (15)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C12-15 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), 1-hexadecanol and C18 (octadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (11) (12) (15)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro

testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C12-15 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, tetradecanol, hexadecanol and octadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (11) (12) (15)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol, dodecanol, C12-16 (types A & B), C12-18 (type B), tetradecanol, hexadecanol and octadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (11) (12) (15)

## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproduction/fertility studies [C12 (dodecanol), C18 (octadecanol) and C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over

the range of linear and essentially linear alcohols.

Data in support of the conclusion that C12-15 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (6) (11) (12) (15)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C12-15 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (11) (12) (15)

### 5.8.3 Toxicity to Reproduction, Other Studies

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### 5.9 Specific Investigations

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### 5.10 Exposure Experience

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### 5.11 Additional Remarks

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(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

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(8) Richterich, K. 2002b. Lial 125-Alcohols, C12-15: Ultimate biodegradability in the closed bottle test. Final report R0200258.

(9) Shell. 1964. Acute toxicity studies on ten materials. Shell proprietary report HSE-63-0004.

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(11) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(12) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(13) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(14) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 66455-17-2
**CAS No.** 66455-17-2
**EINECS Name** Alcohols, C9-11
**EC No.** 266-367-6

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
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**Remark:** Industry Consortium
23-AUG-2005

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20-DEC-2005

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20-DEC-2005

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**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** United Kingdom

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
03-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C9-11 alcohols, CAS 66455-17-2 are >80% linear.

The substance comprises > 95% C9, 10 and 11. Components of even and odd chain length, in the range C8-12 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C9-11 (CA INDEX NAME)
Alc., C9-11
Alcs., C9-11
C9-11 alcohols
Dobanol 91
Dobanol 911
Linevol 911
Neodol 91

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C9-11 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

21-DEC-2005 (6) (14) (19)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

-

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

-

### 1.8.4 Major Accident Hazards

-

### 1.8.5 Air Pollution

-

### 1.8.6 Listings e.g. Chemical Inventories

-

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C9-11 alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

### 1.11 Additional Remarks

-

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

### 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-AUG-2005

## 2.1 Melting Point

**Value:** ca. -21 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Method:** other: ASTM D97
**GLP:** no

**Source:** NOROXO Harnes (NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
05-JAN-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** ca. 216 - 251 degree C at 1013 hPa
**Decomposition:** no

**Method:** other: ASTM D1078
**GLP:** no

**Source:** NOROXO Harnes (NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
05-JAN-2005

**Value:**

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** ca. .831 g/cm³ at 20 degree C

**Method:** other: ASTM D4052
**GLP:** no

**Source:** NOROXO Harnes (NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No reliable measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (18)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .013 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (3)

**Value:** = 2.5 hPa at 55 degree C

**Source:** NOROXO Harnes
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005

**Value:** = 7 hPa at 100 degree C

**Source:** NOROXO Harnes
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005

## 2.5 Partition Coefficient

**log Pow:** = 3.8 - 4.7 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (3)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** 44 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 44 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (3)

**Value:** < .1 vol% at 20 degree C

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** NOROXO Harnes
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 105 degree C
**Type:** closed cup

**Method:** Directive 84/449/EEC, A.9 "Flash point"
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** NOROXO Harnes
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
05-JAN-2005

**2.8 Auto Flammability**

-

**2.9 Flammability**

-

**2.10 Explosive Properties**

-

**2.11 Oxidizing Properties**

-

**2.12 Dissociation Constant**

-

**2.13 Viscosity**

-

**2.14 Additional Remarks**

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (5)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section

1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
11-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance.

The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** TGD Hydrophobics method: Koc = 1430 - 8380
TGD Non-hydrophobics method: Koc = 960 - 2980
TGD Alcohols method: Koc = 90 - 220
SRC PCKOCWIN method: Koc = 50 - 180
**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (5)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 2.97 mg/l related to Test substance
**Degradation:** = 78.9 % after 28 day(s)
**Result:** readily biodegradable

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Other method used: Directive 79/831 EEC, part C, test method C.6, 1985.
**Source:** NOROXO Harnes
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000

CD-ROM. The original report has not been reviewed further because it was not available for review, due to change of business circumstances.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4 - not assignable.

**Flag:** Critical study for SIDS endpoint

07-JAN-2005 (12)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 300 - 2050

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (5)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 2.1 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 2.3 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

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### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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### 4.7 Biological Effects Monitoring

-

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty

acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (11)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Fischer 344
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 5 ml/kg
**Value:** > 5 ml/kg bw

**Method:** other: regulatory procedure
**Year:** 1980
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: There were no mortalities in either test or control animals.

CLINICAL SIGNS: All treated animals had diarrhoea at 0.5 -1.5 hours after dosing, while 4/5 males and all females had polyuria by 24 hours after dosing. Among control animals one female had polyuria. All animals appeared normal by 54 hours post-dosing. The only other observation considered treatment related was hypoactivity in 2 rats during the first 3 hours after dosing. The rats of both treated and control groups gained in body weight over the 14 day observation period and there were no treatment related differences in body weight gain.

NECROPSY FINDINGS: There was no observable pathology in either test or control animals.

POTENTIAL TARGET ORGANS: No conclusions.

SEX-SPECIFIC DIFFERENCES: None

**Source:** Albert 1981a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat F344
- Source: Charles River, Portage, Michigan, US
- Age: Not reported
- Weight at study initiation: males 213.9 + or - 8.1g; females 170 + or - 10.4 g (fasted weights for treated animals)
- Controls: 5M+5F receiving 5 ml/kg distilled water.

ADMINISTRATION:
- Doses: 5 ml/kg Neodol 91
- Doses per time period: single dose
- Volume administered or concentration: 5 ml/kg
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were recorded hourly for 6 hours after dosing then at 24 hours and twice daily throughout the 14 day observation period. Bodyweights were recorded the day before dosing and at 7 and 14 days. A fasted body weight was taken prior to dosing and used for calculation of the dosage. All rats were necropsied at the end of the observation period.

**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position

**Conclusion:** The rat oral LD50 of Neodol 91 is >5 ml/kg (>4000 mg/kg using lowest value of density range 0.8 g/cm3 see chapter 2.3). Signs of intoxication were diarrhoea and hypoactivity. Gross necropsy findings were unremarkable.

**Reliability:** (1) valid without restriction
Comparable to guideline study

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (1)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Inhalation: Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category from C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the substantially saturated vapour concentration. This includes data for C8 (1-octanol), C8-10, C9 (1-nonanol), C10 (1-decanol), C6-12 and C11 (undecanol) alcohols in support of the statement that C9-11 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the substantially saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of systemic toxicity is based are either comparable to guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (20)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 8
**Vehicle:** other: undiluted
**Doses:** 2 ml/kg
**Value:** > 1660 mg/kg bw

**Method:** other: in house protocol
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure and 14 day observation period. The dermal LD50 is therefore >2 ml/kg, this is equivalent to 1660 mg/kg using a density of 0.83 for conversion.

APPLICATION SITE: There was minimal skin irritation at the 24 hour period for both intact and abraded skin. Mean erythema and oedema scores for intact skin were 1.9 and 1.1 respectivley compared to 0.2 and 0.1 in the controls. For abraded skin erythema and oedema scores were 2 and 1 respectively with control values of 0.6 and 0.1. No irritation was evident at 14 days.

CLINICAL SIGNS: There were no treament related signs of toxicity. Bodyweights in treated animals were comparable to those of controls.

NECROPSY FINDINGS: The presence of white flaky material at the application site was the only remarkable finding.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Albert, J.R. 1981b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Camm Research Institute, Wayne, New Jersy, USA
- Age: Not reported
- Weight at study initiation: average weight 3.10 kg
- Group size: 4M+4F
- Controls: 4M+4F

ADMINISTRATION: 24 hour occluded application to intact and abraded skin.
- Area covered: 4X4 inches
- Occlusion: Gauze plus impervious wrap (Saran) and elastic bandage.
- Total volume applied: 2 ml/kg
- Doses: 2 ml/kg
- Removal of test substance: Remaining material removed using a moist towel.

EXAMINATIONS: Observations for mortality and clinical signs were made at 1,2,4,6 and 24 hours after application and then twice daily through out the 14 day observation period. Each exposure site was scored (Draize) for degree of irritation immediately on removal of the dressings and prior to termination on day 14. Body weights were measured on days -1, 0, 7 and 14. Survivors were necropsied at the end of the observation period.

STATISTICAL METHODS: These included calculation of mean and standard deviation. Determination of the significance of bodyweight changes compared to controls was made using an independent T-test.

**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position

**Conclusion:** The rabbit dermal LD50 (24 occlusive exposure) for Neodol 91 is >1660 mg/kg. Other than irritation at the application site, reversible within the 14 day observation period, there were no other signs of toxicity.

**Reliability:** (1) valid without restriction
Comparable to guideline study

**Flag:** Critical study for SIDS endpoint

28-OCT-2004 (2)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**PDII:** 4.2
**Result:** irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Mean 24 + 72 hour score for 6 animals intact skin 2.67, abraded skin 2.75.
- Oedema: Mean 24 + 72 hour score for 6 animals intact skin 1.46, abraded skin 1.54.

REVERSIBILITY: At 7 days all the application sites had developed eschar (scored as 4) so the effects had increased over the period of the study. PII 4.2.

**Source:** Cagen 1981c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: male + female
- Source: Camm Research Institute, New Jersey, USA
- Weight at study initiation: 2.2 - 3 kg
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 1 inch square
- Occlusion: Occlusive
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 24 hours to intact and abraded skin (2 sites each per animal)
- Postexposure period: 7 days

- Removal of test substance: Removed using a moist towel.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 48 hours after exposure and at 7 days.

**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position

**Conclusion:** Neodol 91 was a skin irritant following 24 hour occlusive application to rabbit skin according to both EU and GHS classification systems.

**Reliability:** (1) valid without restriction
Comparable to guideline study

**Flag:** Critical study for SIDS endpoint

28-OCT-2004 (9)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand White rabbits
**Concentration:** undiluted
**Dose:** .1 ml
**Exposure Time:** .5 minute(s)
**Comment:** other: rinsed and unrinsed
**No. of Animals:** 9
**Vehicle:** none
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour) unrinsed
- Cornea: individual scores 4 rabbits 0, 1 rabbit 0.33, 1 rabbit 0.67. (group mean score 0.17)
- Iris: Individual scores all 0 (group mean score 0)
- Conjunctivae (Redness): individual scores 1, 0, 1, 0.33, 0, 0.67 (group mean score 0.5)
- Conjunctivae (Chemosis): individual scores 3 rabbtis scored 0, 0.67, 1.3, 0.3 (group mean score 0.39)
- Overall irritation score: Maximum mean total score 8.8 at 24 hours after instillation.

AVERAGE SCORE (24+48+72 hour) rinsed
- Cornea: individual scores all 0 (group mean score 0)
- Iris: Individual scores all 0 (group mean score 0)
- Conjunctivae (Redness): individual scores 0.3, 0, 0.3 (group mean score 0.2)
- Conjunctivae (Chemosis): individual scores 0.3, 0, 0.3 (group mean score 0.2)
- Overall irritation score: Maximum mean total score 4.7 at 1 hours after instillation.

REVERSIBILITY: All scores were 0 at 7 days both rinsed and unrinsed.

OTHER EFFECTS: Conjunctival discharge reported in some rabbits up to 48 hours post instillation (unrinsed) and 1 hour after

instillation (rinsed).
**Source:** Cagen 1981a
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male (6) and female (3)
- Source: Camm Research Institute, USA
- Weight at study initiation: 2.1 - 2.7 kg
- Number of animals: 3M+3F unrinsed; 3M rinsed.
- Controls:

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: Draize, 1963 plus Kay & Callandra 1962 (modified)
- Observation period: 7 days
- Tool used to assess score: No data.

**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position
**Conclusion:** Neodol 91 is not an eye irritant by either EU or GHS criteria.
**Reliability:** (1) valid without restriction
Comparable to guideline study
**Flag:** Critical study for SIDS endpoint
02-AUG-2005 (7)

## 5.3 Sensitization

**Type:** Buehler Test
**Species:** other: Duncan Hartley albino guinea pig
**Concentration 1st:** Induction 1 % occlusive epicutaneous
**2nd:** Challenge 1 % occlusive epicutaneous
**No. of Animals:** 10
**Vehicle:** other: absolute ethanol
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** One male animal died during the study. Gross necropsy determined that it was not related to the test material. There was slight irritation in the test group which decreased over the 5 week test period from 0.38 at week 1 to 0.00 at week 5. Neodol 91 is a non-sensitizer.
RESULTS OF PILOT STUDY: No irritation with the 1% solution, significant irritation with the 50 and 100% solutions.

RESULTS OF TEST
- Sensitization reaction: There were no positive responses at challenge in the test group. Slight irritation was observed during the induction period. The positive controls showed a significant response at challenge with all test sites showing

an increased degree of irritation.

Average irritation at challenge for the treated group was 0, positive controls were 1.55, vehicle controls 0.08 and irritation controls (challenge application only) 0.13.

- Clinical signs: One animal died in the positive control group but this was not attributable to treatment.

- Rechallenge: Not required.

**Source:** Cagen 1981b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: Dunkin-Hartley
- Sex: male & female
- Source: Camm Research Laboratoires, New Jersey, USA
- Weight at study initiation: 500-600g
- Number of animals: 5M+5F treated
- Controls: 5M+5F irritation, vehicle and positive controls.

ADMINISTRATION/EXPOSURE
- Study type: Buehler, non-adjuvant.
- Preparation of test substance for induction: in ethanol
- Preparation of test substance for challenge: in ethanol
- Induction schedule: Topical application of 0.5 ml test solution (occlusive) one day a week, 6 hours/day for 3 consecutive weeks.
- Concentrations used for induction: 1%
- Challenge schedule: Topical application of 0.5 ml test soln. (occlusive) 2 weeks after the last sensitising dose.
- Concentrations used for challenge: 1%
- Rechallenge: No
- Positive control: 2,4-dinitrochlorobenzene 0.1% in diethyl ether.

EXAMINATIONS
- Grading system: Draize
- Pilot study: 1M+1F at each of 3 concentrations 100, 50 or 1% in ethanol.

**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position

**Conclusion:** Neodol 91 is not a skin sensitiser in guinea pigs when tested using the Buehler method.

**Reliability:** (1) valid without restriction
Comparable to guideline study

**Flag:** Critical study for SIDS endpoint

05-DEC-2005 (8)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** rat **Sex:** male/female
**Strain:** Fischer 344
**Route of administration:** other: Atmosphere containing saturated vapor
**Exposure period:** 9-days over a 12-day period
**Frequency of treatment:** 6-hours/day
**Post exposure period:** None
**Doses:** 0.0 and 158 mg/m3
**Control Group:** yes, concurrent no treatment

**NOAEL:** > .158 mg/l

**Method:** other: see text
**Year:** 1982
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were no significant differences between test and control group for any of the parameters evaluated. NOAEL 0.158 mg/l (saturated vapour concentration).
**Source:** Darmer and Wimberly 1982.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Weight at study initiation: males 253-276 g; females 147-179 g
- Number of animals: 8M+8F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 9 days
- Type of exposure: inhalation, whole body
- Post exposure period: none
- Vehicle: Air
- Concentration in vehicle: nominally 0.158 mg/l (saturated vapours)
- Doses: 0, 0.158 mg/l

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs/mortality: Before, during and after exposure on exposure days, twice daily on non-exposure days.
- Body weight: Prior to each exposure and at necropsy.
- Haematology: At sacrifice, haematocrit, Hb, RBC, total & differential WBC, platelets
- Biochemistry: Serum glucose, urea nitrogen, total protein, albumin, sodium , potassium, phosphorus, calcium , cholesterol , ALAT, ASAT, alkaline phosphatase, total bilirubin.
ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: full necropsy, organ weights recorded to liver, kidneys, lungs, heart, liver, kidneys, spleen & stomach plus any abnormalities.
- Microscopic: Representative sections from the respiratory tract and any lesions considered significant.
STATISTICAL METHODS: body weight changes by covariance analysis. Organ weights, haematology and clinical chemical parameters, variance, covariance or non-parametric methods as appropriate.
**Test substance:** C9-11 alcohols Cas# 66455-17-2 (Neodol 91) 84% linear monobranched at the 2 position
**Reliability:** (2) valid with restrictions
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
02-AUG-2005 (10)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5

to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C9-11 alcohols are available from studies of reliability 1 or 2 for 1-hexanol [Ames], 1-octanol [Ames], 1-decanol [Ames], C6-12 (type C) [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion] and 1-dodecanol (supporting) [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of systemic toxicity is based are either guideline or comparable studies or publications with sufficient detail for assessment.

25-OCT-2005 (16) (20)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either comparable to guideline studies or publications with sufficient detail for assessment.

25-OCT-2005 (16) (20)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproduction screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C9-11 alcohols are not

expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of systemic toxicity is based are either comparable to guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (16) (17) (20)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C9-11 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for developmental toxicity is based are either guideline or similar studies or publications with sufficient detail for assessment.

12-SEP-2005 (16) (17) (20)

### 5.8.3 Toxicity to Reproduction, Other Studies

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### 5.9 Specific Investigations

-

### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

**Type:** other: comment on entries in RTECS 2004

**Remark:** The values reported are for Linevols 79 and 911 which correspond to Cas no. 68603-15-6.

28-OCT-2004 (15)

**Type:** other: comment on existing Iuclid

**Remark:** The data provided in this data set relates to individual C9 and 11 oxo alcohols. None of this is included here.

02-AUG-2005 (13)

(1) Albert, J.R. 1981a. Acute oral toxicity of NEODOL 91 alcohol in the rat. Westhollow Research Center. Shell Project Number 65102.

(2) Albert, J.R. 1981b. Acute dermal toxicity of NEODOL 91 alcohol in the rabbit. Westhollow Research Center. Shell Project Number 65102.

(3) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(4) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(5) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(6) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(7) Cagen, S.Z. 1981a. Eye irritation of NEODOL 91 alcohol. Shell Project No. 65102.

(8) Cagen, S.Z. 1981b. Guinea pig skin sensitization study of NEODOL 91 alcohol. Shell Project No. 65102. Regulatory information record. WRC RIR-162.

(9) Cagen, S.Z. 1981c. Primary skin irritation of NEODOL 91 alcohol. Shell Project No. 65102. WRC RIR-161

(10) Darmer, K.I. and Wimberly, H.C. 1982. Acute inhalation study in rats with Neodol 91 alcohol vapor. WRC RIR-262, Westhollow Research Center, Houston, TX.

(11) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(12) Exxon Biomedical Sciences, Inc. (1992). Final Report. "Ready biodegradability: Closed Bottle Test (Unacclimated Seed)". EBSI document # 92MRL 95.

(13) Iuclid 2000 European Commission - European Chemicals Bureau C9-11 alcohols Cas# 66455-17-2

(14) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(15) RTECS on line 2004 Cas 66455-17-2

(16) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by

consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(17) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(18) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(19) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(20) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 67762-25-8
**CAS No.** 67762-25-8
**EINECS Name** Alcohols, C12-18
**EC No.** 267-006-5
**TSCA Name** Alcohols, C12-18

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

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03-AUG-2005

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**Town:** 20005 Washington DC
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**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
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**Remark:** Consortium Member
20-DEC-2005

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20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. Dave Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
03-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

03-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C12-18 alcohols, CAS 67762-25-8 are 100% linear.

The substance comprises >95% C12, 14, 16 and 18. Components of even chain length, in the range C8-C20 are present.

Commercial products marketed under this CAS number fall into two types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A and Type B.

Type A products are 100% linear. The substance comprises >50% C12 and C14; >10% C16 and C18. Components of even chain length, in the range C8-C20 are present.

Type B products are 100% linear. The substance comprises >10% C12 and C14; >60% C16 and C18. Components of even chain length, in the range C12-C20 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C12-18 (CA INDEX NAME)
Alfol 1218
Alfol B
C12-18 alcohols
Lorol

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C12-18 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:
USA: ca. >5 - 250 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 - 500 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes,

exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.
21-DEC-2005 (4) (23) (28)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or

other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (30)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-18 alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

03-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

03-AUG-2005

## 2.1 Melting Point

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Solidification range 25-28 degr. C.
**Source:** Henkel KGaA Duesseldorf
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.
**Flag:** Critical study for SIDS endpoint
05-JAN-2005 (6)

**Remark:** Solidification range 18-23 degr. C.
**Source:** Henkel KGaA Duesseldorf
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number. The original reference is secondary literature and therefore the reliability of the data cannot be verified.
17-OCT-2005 (6)

**Remark:** Solidification range 20-28 degr. C.
**Source:** Henkel KGaA Duesseldorf
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number. The original reference is secondary literature and therefore the reliability of the data cannot be verified.
17-OCT-2005 (6)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** = 260 - 350 degree C at 1013 hPa

**Method:** other: DIN 51751
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number. The original reference is secondary literature and therefore the reliability of the data cannot be verified.
**Flag:** Critical study for SIDS endpoint
05-JAN-2005 (24)

**Value:**

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** = .81 - .82 g/cm³ at 40 degree C

**Method:** other: DIN 51757 Verf. B
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
**Flag:** Critical study for SIDS endpoint
05-JAN-2005 (24)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** It is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
21-OCT-2005 (27)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00026 - .0016 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.0016 value hPa
Type B: 0.00026 value hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 5.4 - 7.2 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .35 - 1.7 mg/l at 25 degree C

**Method:** other: (calculated) partition model

**Year:** 2005
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 1.7 mg/l at a loading rate of 100 mg/l
Type B: 0.35 mg/l at a loading rate of 1000 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
19-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 140 degree C
**Type:** closed cup

**Method:** other: DIN 51758
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
05-JAN-2005 (24)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable

11-OCT-2005 (21)

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (21)

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (21)

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.

**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section

1.0.4 for a list of long chain alcohols CAS).
This conclusion applies to both compositional Types.
11-SEP-2005

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**
TGD hydrophobics method: Koc = 27600 - 839000
TGD Non-hydrophobics method: Koc = 6420 - 57400
TGD Alcohols method: Koc = 389 - 2010
SRC PCKOCWIN method: Koc = 327 - 12900

These values apply to both compositional Types.

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Test substance:** As prescribed by section 1.1-1.4
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent from municipal sewage treatment plant (appr. 1000 - 100,000 cells/ml)
**Concentration:** 2 mg/l related to Test substance
5 mg/l related to Test substance
**Contact time:** 29 day(s)
**Degradation:** = 79 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**
7 day(s) = 58 %
14 day(s) = 73 %
21 day(s) = 75 %
28 day(s) = 79 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Inert nonylphenol ethoxylated propoxylated (NP+9.5 EO+5PO) was used at a 1:1 ratio to emulsify poorly soluble test substance. Degradation rate of test substance was corrected by oxygen uptake of blank inoculum and emulsifier control.

Oxygen concentrations were determined by iodometric titration according to Winkler.

The validity criteria were fulfilled: (1) results of parallel assays did not differ from each other by more than 20%, (2) degradation of reference substance reached pass level within 14 days, (3) oxygen depletion in inoculum blank did not exceed 1.5 mg O2/l after 30 days. (4) residual oxygen concentration did not fall below 0.5 mg/l at any time (only for 2 mg/l; insufficient residual oxygen at 5 mg/l).

**Result:** Kinetic of control substance:
7 days = 76%
14 days = 78%
21 days = 76%
28 days = 88%
Two concentrations of test substance were tested: 2 mg/l and 5 mg/l. The degradation values reported are for the 2 mg/l concentration. The 5 mg/l test concentration attained 56% degradation, but had insufficient residual dissolved oxygen content, therefore the reuslts are not considered valid. At the 2 mg/l concentration, the test substance degraded >60% over the test period. Insufficient information is reported to confirm whether the 10 day window criterion was met but since 58% degradation was attained by day 7, the substance is considered to be readily biodegradable.

**Test condition:** Concentration of effluent: 1ml/l
Approx. 1000 - 100,000 cells/ml
Test volume: 300 ml
Temperature: 20 +/- 1 C
pH: no data

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (18)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Degradation:** after 28

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** EG-RiLi 84/449 Anh.V C4-E
**Remark:** Hemmtest: keine Hemmung des FA 8 EO Abbaus. nur Hemmtest
**Source:** Henkel KGaA Duesseldorf
**Test substance:** Active Matter = 100 %

It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (10) (14)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 100 mg/l
**Degradation:** = 16 % after 28 day(s)
**Result:** other: moderately biodegradable

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 100 mg/l referring to Chemical oxygen demand: 16% with parameter % BSB/CSB
**Test substance:** Active Matter = 100 %
It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (8) (12)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 100 mg/l
**Degradation:** = 35 % after 28 day(s)
**Result:** other: moderately biodegradable

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 100 mg/l referring to Chemical oxygen demand: 35% with parameter % BSB/CSB
**Test substance:** Active Matter = 100 %
It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (9) (13)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage

**Concentration:** 100 mg/l
**Degradation:** = 0 - 81 % after 28 day(s)
**Result:** other: readily degradable

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Remark:** In einem schwach beimpften Parallelversuch ( OECD 301D-Animpfung = 5ml Kläranlagenablauf/l) erreichte das Prüfmuster 80% BSB/ThSB nach 28 Tage
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 100 mg/l referring to ThSB: 81% with parameter % BSB/ThSB
#2: 0 mg/l referring to ThSB: 0% with parameter % BSB/ThSB
**Test substance:** Active Matter = 100 %
It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (7) (11) (15)

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, though the ten-day window may not be met. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to both compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 7200 - 43800

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

This conclusion applies to both compositional Types.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 1.2 - 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 1.2 mg/l
Type B: >100 mg/l (i.e. predicted to be non-toxic at the limit of solubility)
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** = 40
**Limit Test:** no

**Method:** other: EU guideline 92/69/EWG
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Nominal test concentrations were 10, 30, 100, 1000, and 3000 mg/L. No solvent was used. Instead, the water accommodated

fraction (WAF) was used in the test chambers. Measured concentrations in samples collected from the 10 and 100 mg/L chambers were less than 1% of nominal. The solubility of the lowest carbon chain length in this compound, C12, is 3 mg/l, therefore the EC50 was greater than the solubility limit.

**Result:** RESULTS: EXPOSED
EL0 = 10 mg/l
EL50 = 40 mg/l
EL100 = >3000 mg/l
Based on nominal loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Kirch 1998a

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: BioInternational B.V., NJ Horn, NL
Age: 6-24 hours old
Feeding: Green algae during 6 hours prior to testing
Pretreatment: M4 medium / 20oC / 16h light - 8h dark
Feeding during test: No feeding according to EU guideline
Control group: 1 group (2 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Not reported
DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: 10, 30, 100, 1000, 3000 mg/L
Renewal of test solution: None
Exposure vessel type: 100 ml beakers covered with clockglasses
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20.8-20.9 C
Dissolved oxygen: 99.2%
pH mean: 7.9
Adjustment of pH: not reported
Intensity of irradiation: approx. 900 lux
Photoperiod: 16 hours light/ 8 hours darkness
TEST PARAMETER: Immbolization
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Yes (fluid chromatography of dichloromethane extract)
Measured concentrations of C12, C14, C16 and C18 were between 0.003 and 0.025 mg/l at 48 hours for 10 and 100 mg/l dose groups.

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (22)

**Unit:** mg/l **Analytical monitoring:** no

**EC50:** = .5 - 17 calculated

**Method:** other

**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.5 mg/l
Type B: 17 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. 10 - 100

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a

range.

For compositional Type B for this substance, for which a prediction of algal toxicity is required, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The value obtained by prediction is:
Type B: 10 - 100 mg/l

For Type A, a reliable measurement is available. Therefore, no estimation is made.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

**Species:** other algae: Pseudokirchneriella subcapitata
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = 1.2
**ErL50 :** = 7.5
**EbL50 :** = 2.3
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2003
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** WAFs were prepared by loading test medium with the respective amount of the test item. After stirring the contents were left to settle for 24h. The WAFs were filtered prior to use through a non polar filter (0.2 um Millex FG, 50 mm, Millipore).

**Result:** RESULTS: EXPOSED
NOEL = 1.2 mg/l
LOEL = 2.4 mg/l
ErL10 = 1.9 mg/l
ErL50 = 7.5 mg/l
EbL10 = 0.8 mg/l
EbL50 = 2.3 mg/l
Based on loading rates

**Source:** Wenzel 2003.

**Test condition:** TEST ORGANISMS
Strain: Pseudokirchneriella subcapitata
Supplier: Institute for plant physiology, University Gottingen
Pretreatment: Not reported
Controls: 1 control group (3 replicates)
Test medium: Water Accommodated Fractions
Vehicle, solvent: None
Concentration of vehicle, solvent: None
STABILITY OF TEST CHEMICAL SOLUTIONS
Considered stable under normal conditions of use

DILUTION WATER
Source: Purified water using an ECGA UHQ/PS water purification system
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Reciprocal conductivity > 18 Mohm*cm
TEST SYSTEM
Loading rates: 0.6, 1.2, 2.4, 4.8 and 9.6 mg/l
Exposure vessel type: 250 mL conical glass flasks covered with silicone-sponge caps
Number of replicates: 3
Initial cell concentration: 10,000 cells/ml
Test temperature: 21 - 23
Dissolved oxygen: Not reported
pH mean: 7.4 - 9.8
Adjustment of pH: None
Intensity of irradiation: 6822 - 8363 lux
Photoperiod: not reported
TEST PARAMETER: growth rate and biomass
MONITORING OF TEST SUBSTANCE CONCENTRATION: During the test the stability of the fatty alcohols was examined in additionally prepared replicates of WAFs of a low and a high loading rate (1.2 and 9.6 mg/l) with and without algae. At test end, C10 FA concentrations were comparable with the initial concentrations. C12 FA concentrations were between 71% and 89% of the concentrations at test start. C14 FA were below the LOQ in all test vessels during the test.

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (31)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

## 4.6.3 Toxicity to Soil Dwelling Organisms

-

## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.

Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (5)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: aqueous suspension
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died during the 14 day observation period.

CLINICAL SIGNS: Directly following administration of the test substance all the animals showed piloerection and slight sedation. These effects vanished within 24 hours. No other effects appeared in the 14 day observation period. The animals gained in bodyweight over the observation period.

NECROPSY FINDINGS: Nothing remarkable in the males. In the females the gastric mucosa was swollen.

POTENTIAL TARGET ORGANS: Possible effect on the gastric mucosa in females.

SEX-SPECIFIC DIFFERENCES: Effect on gastric mucosa observed only in females.

**Source:** Henkel KGaA 1981e
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: rat (Wistar)
- Source: Winkelmann, Hannover, Germany
- Weight at study initiation: average weight males 156g, females 137g
- Group size: 5M+5F fasted
- Controls: No

ADMINISTRATION:
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 20 ml/kg of a 25% aqueous suspension.
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs were observed at 1, 4 and 24

hours after dosing and then daily. Body weights were recorded prior to dosing and at 24 hours, 1 week and 2 weeks after dosing. All survivors were subject to gross necropsy at the end of the observation period.

**Test substance:** Tradename Lorol 12-18 technical C12-18 alcohols Type A

**Conclusion:** The rat oral LD50 for Lorol C12-18 is >5000 mg/kg. Signs of intoxication were slight sedation and piloerection. Necropsy revealed swelling of the gastric mucosa in females only.

Study cited in Iuclid 2000, there appear to be two entries forhte same study both citing the archive number 937.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (16) (20)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C10 (1-decanol), C12 (1-dodecanol), C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18 and C20 (eicosanol) alcohols in support of the statement that C12-18 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (25) (29)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20) including data for C12 (1-dodecanol), C16 (1-hexadecanol), C12-16 and C20 (eicosanol) alcohols which support the statement that C12-18 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (25) (29)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

### 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Result:** highly irritating
**EC classificat.:** irritating

**Method:** Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"
**Year:** 1992
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of unpublished Henkel data Steiling, W. Report no. 920073, 1992. Carried out according to Directive 84/449/EEC, B4 no other details given. Reported as highly irritating.
**Source:** Iuclid 2000
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Kokoslorol C12-18, C12-18 alcohols insufficient compositional information to ascribe a type.
**Reliability:** (4) not assignable
Secondary reference only.
25-JUL-2005 (20)

**Species:** human
**Exposure:** Open
**No. of Animals:** 10
**Vehicle:** no data
**Result:** irritating
**EC classificat.:** irritating

**Method:** other: Burchardt test
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Summary report of a human volunteer study unpublished Henkel data (Matthies W. Report no. 880692, 1988). This was an open epicutaneous test, no further test details were given. The product was reported to produce slight redness disappearing up to 40 minutes following the last application.

Iuclid 2000 also refers to the publication by Kaestner, J. Soc. Cos. Chem. 28:741-754, 1977 in relation to this study, however there appears to be no mention of C12-18 alcohols in the publication. There appears to be a second reference to similar data in Iuclid 2000 referring to unpublished Henkel data from the same report as above but giving a classification

of slightly irritating.
**Source:** Iuclid 2000
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Lorol 12-18 technical C12-18 alcohols Type A
**Reliability:** (4) not assignable
Secondary reference only.
25-JUL-2005 (20)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel refering to Archive no. 880232. This skin irritation test in the rabbit was carried out to Directive 84/449/EEC, B4. The test material was not considered an EU irritant but the descriptive classification was irritant. No further details given.
**Test substance:** C12-18 alcohols insufficient compositional information to ascribe type.
**Reliability:** (4) not assignable
Secondary reference.
25-JUL-2005 (20)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA archive no. RT 920073. Rabbit irritation study according to Directive 84/449/EEC, B4. The test substance is described as highly irritating and EU classified as irritating.
**Test substance:** C12-18 alcohols insufficient compositional information to ascribe type.
**Reliability:** (4) not assignable
Secondary reference.
25-JUL-2005 (20)

### 5.2.2 Eye Irritation

**Remark:** Unpublished data from Henkel KgaA archive TBD 880614.

Rabbit eye irritation test to OECD guide-line 405. The test substances is described as slightly irritating and EU classified as not iritating. No further details available.
**Test substance:** As prescribed by 1.1 - 1.4 (insufficient compositional information to ascribe types)
**Reliability:** (4) not assignable
Secondary reference.
14-SEP-2005 (20)

### 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C6 (hexanol), C10-16 alcohols, C12 (dodecanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C12-18 alcohols are not expected to be skin

sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are either guideline studies or comparable or publications with sufficient detail for assessment.
05-DEC-2005 (25) (26) (29)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C12-18 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (25) (26) (29)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Bacterial reverse mutation assay
**System of testing:** Salmonella typhimurium strains TA 100, TA 1535, TA 1537, TA 1538, TA 98
**Concentration:** 4, 20, 100, 500, 2500 ug/plate
**Cytotoxic Concentration:** 500 - 2500 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 471
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: There was no increase in reverse mutation rate in any of the test strains at any dose level, positive controls gave appropriate responses in terms of increased mutation.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: Toxicity observed at the two highest dose levels (2500 ug/plate and/or 500 ug/plate as evidenced by partial or complete reduction in numbers of revertants.

**Test condition:** METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Duplicates.
- Application: Plate incorporation.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

**Test substance:** Tradename Lorol C12-18 C12-18 alcohols Type B

**Conclusion:** The C12-18 alcohol Lorol C12-18 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Cytotoxicity was evident in most strains at 500 and 2500 mg/kg.

This study is cited in Iuclid 2000.

**Reliability:** (2) valid with restrictions
comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (17)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol, dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of

this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline or similar studies or publications with sufficient detail for assessment.

14-SEP-2005 (19) (25) (26) (29)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C12-18 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol), C22 (docosanol) and data from supporting substances 1-hexanol-2-ethyl, isoamyl alcohol and C18 (octadecanol)

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (25) (26) (29)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols

there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C12-18 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are either comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (25) (26) (29)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(6) Dehydag catalog fatty alcohols, Henkel KGaA (1993)

(7) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No 9701848 2

(8) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE 910231

(9) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE 920041

(10) Henkel KGaA, unpublished data, Archive No./BIAS-No./Test No. PE 920064

(11) Henkel KGaA, unpublished data, Final report 9700631

(12) Henkel KGaA, unpublished data, Final report RE 920029

(13) Henkel KGaA, unpublished data, Final report RE 920103

(14) Henkel KGaA, unpublished data, Final report RE 920123

(15) Henkel KGaA, unpublished data, Protocol LIMS

(16) Henkel KGaA. 1981e. Alcohols, C12-18: Evaluation of acute oral toxicity. Unpublished data, Report No. R 9500187 and summary 1999.

(17) Henkel KGaA. 1982c. Alcohols, C12-18: Evaluation of mutagenicity. Unpublished data, Report No. 820116.

(18) Henkel KGaA. 1992b. Lorol C12-C18: Bewertung der biologischen Abbaubarkeit im GF-Test (Aerobic biodegradation: Closed bottle test). Biological Research and Product Safety/Ecology: test substance registration No. SAT910720, test run No. 1012. Report-Nr. RE 920245. 18 Dezember 1992.

(19) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(20) Iuclid 2000 European Commission - European Chemicals Bureau Alcohols C12-18 Cas# 67762-25-8

(21) IUCLID data sheet. 1995d. C12-18.

(22) Kirch, A. 1998a. Alkohole, C12-18 akute Daphnientoxizitat. Henkel Report No. R9800103.

(23) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(24) Safety data sheet Henkel KgaA

(25) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(26) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(27) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(28) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(29) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(30) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

(31) Wenzel A., (2003), Draft Study Report: Alga, Growth Inhibition Test, Effects of Water Accommodated Fractions (WAF) of Fatty Alcohols on the growth of Pseudokirchneriella subcapitata, Cognis Deutschland GmbH & Co. KG, Dusseldorf, Germany

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 67762-27-0 |
| **CAS No.** | 67762-27-0 |
| **EINECS Name** | Alcohols, C16-18 |
| **EC No.** | 267-008-6 |
| **TSCA Name** | Alcohols, C16-18 |
| | |
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| | |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| | |
| **Memo:** | MERGED JAN 2006 |
| | |
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **28-DEC-2005** |
| | |
| **Number of Pages:** | **56** |
| | |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

03-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. Dave Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

### 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

### 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium

members, those identified as C16-18 alcohols, CAS 67762-27-0 are 100% linear (or unstated).

The substance comprises <10% C14, >=90% C16 and 18. Components of even chain length, in the range C12-C20 are present.

05-AUG-2005

### 1.1.2 Spectra

**Remark:** Not required

11-AUG-2003

### 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C16-18 (CA INDEX NAME)
Cetearyl alcohol
Cetostearyl alcohol
Cetylstearyl alcohol
Cire algonol CS
Cire deLanol ST
Conol 30OC
Crodacol SCB
Cyclochem emulsion wax
Dehydag wax N
Epal 1618
Hydrenol D
Hydrenol DV
Hydrenol MY
Hyfatol CS
Hyfatol CS 50
Hyfatol CS/EP
Kalcohl 68
Kalcohl 6850
Kalcohl 6870
Kalcohl 86
Kalcohl 8665
Kalcohl 8688

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

### 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C16-18 alcohols.

Composition is described in section 1.1.1, General Substance

Information.
05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >250 - 500 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >500 000 - 1 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.
21-DEC-2005 (4) (24) (30)

## 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

## 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

## 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

## 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

**Use category:** 15 Cosmetics
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 41 Pharmaceuticals
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available
19-SEP-2005

**Use category:** 50 Surface-active agents
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (32)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C16-18 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
11-AUG-2003

## 2.1 Melting Point

**Value:** ca. 49 - 56 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Method:** other
**GLP:** yes

**Source:** UNION DERIVAN S.A. VILADECANS (NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

**Remark:** Solidification range: 48 - 52 degr. C
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (26)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** ca. 300 - 360 degree C

**Method:** other
**GLP:** yes

**Source:** UNION DERIVAN S.A. VILADECANS(NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

**Value:** = 310 - 360 degree C at 1013 hPa

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (26)

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** ca. .8 g/cm³ at 20 degree C

**Method:** other
**GLP:** yes

**Source:** UNION DERIVAN S.A. VILADECANS(NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

**Type:** density
**Value:** = .805 - 815 g/cm³ at 60 degree C

**Method:** other: DIN 51757 B

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (26)

**Value:** = .81 - .82 at 60 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (23)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000013 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** 6.7 - 7.2 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .03 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.030 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Solubility in:** Water
**Value:** .283 at 20 degree C
**Descr.:** not soluble

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005 (26)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** > 160 degree C
**Type:** open cup

**Method:** other
**GLP:** yes

**Source:** UNION DERIVAN S.A. VILADECANS (NO REFERENCE GIVEN)
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005

**Value:** ca. 170 degree C

**Type:** open cup

**Method:** other: DIN 51758/ISO 2719
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
05-JAN-2005 (26)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (23)

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (23)

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (23)

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.

**Flag:** Critical study for SIDS endpoint
07-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4.

However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure).

Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint

13-SEP-2005

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance.

The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**
TGD Hydrophobics method: Koc = 96500 - 839000
TGD Non-hydrophobics method: Koc = 30100 - 57400
TGD Alcohols method: Koc = 1240 - 2010
SRC PCKOCWIN method: Koc = 3790 - 12900

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods

28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent from predominantly domestic sewage treatment plant
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 81 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**
7 day(s) = 58 %
14 day(s) = 73 %
21 day(s) = 77 %
28 day(s) = 81 %
**Control Subst.:** other: not reported

**Method:** other: ISO 10708 (BODIS)

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken.
**Remark:** This information is from a 1 page summary of the full report. It states that test chemical concentration is 100 mg COD/l in the test procedure, however is also stated as 50 mg COD/l in the results section. No information is given on the validity criteria.
**Result:**
The substance degraded >60% over the test period. Insufficient information is reported to confirm whether the 10 day window criterion was met but since 58% degradation was attained by day 7, the substance is considered to be readily biodegradable.
**Test condition:** Inoculum concentration: not reported
Test volume: not reported
Temperature: not reported
pH: not reported
**Reliability:** (4) not assignable
Summary report only available for review. No information reported on reference material or validity criteria for the test.
**Flag:** Critical study for SIDS endpoint
13-SEP-2005 (20)

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 46 day(s)
**Degradation:** = 21 - 65 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 12 day(s) = 3 - 10 %
19 day(s) = 7 - 21 %
28 day(s) = 21 - 65 %
46 day(s) = 55 - 91 %
**Control Subst.:** other: Sodium acetate

**Method:** other: Sturm 1973
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** This test method corresponds to OECD 301B.
**Remark:** The following validity criteria were met:
(1) the blanks were valid for this test, the maximum milligrams of carbon dioxide were well within the 40 mg/l range (13.5-18.8 mg/l),
(2) the reference substance reached the pass level within 14 days.

Duplicate assays were performed, although the samples were prepared differently. The first sample was prepared by direct addition of a single piece of solid material to the test

vessel, while the second was added using a heated dropper to produce round solid droplets. Results were not within +/- 20% for the two samples.

**Result:** Kinetic of control substance:
8 days = 57.0%
14 days = 72.3%
22 days = 82.3%
28 days = 83.0%
The test substance did not meet the '10-day window' rule for ready biodegradation. The test substance required 5 extra days for a total of 15 days to reach 60% of maximum theoretical carbon dioxide production. The reference substance Sodium acetate degraded by 84% after 28 days.

**Test condition:** Inoculum concentration: 3 - 5 g/l suspended solids, diluted 200 ml to 3 litres in mineral medium.
Test volume: 3000 ml
Temperature: not reported
pH: not reported

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with higher degradation rates are available.

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (25)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 50 mg/l
**Degradation:** = 56 - 62 % after 28 day(s)

**Method:** ISO Draft "BOD Test for insoluble substances"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Remark:** Abbauhemmtest: keine Effekte. Animpfung 10 fach höher als Routine BLOK Test (hohe Eigenzehrung IZK) parallel wurde ein Hemmtes durchgeführt CSB= 1.97mg O2/mg AS BSBT=3.19mg O2/mg AS
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 56% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 62% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 66% with parameter % BSB/CSB

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

28-SEP-2005 (12) (14) (18)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 50 mg/l
**Degradation:** = 81 - 100 % after 28 day(s)
**Result:** other: readily degradable

**Method:** ISO Draft "BOD Test for insoluble substances"

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** two phase closed bottle test
**Remark:** zusätzlich Abbauhemmtest: keine Effekte.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 81% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 100% with parameter % BSB/ThSB
#3: 50 mg/l referring to Chemical oxygen demand: 79% with parameter % BSB/CSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (13) (14) (19)

**Type:** aerobic
**Inoculum:** other: municipal sewage treatment plant effluent
**Concentration:** 50 mg/l
**Degradation:** = 73 - 82 % after 30 day(s)

**Method:** other: AWU-Test. Closed bottle test for poorly water-soluble
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parameter: % BOD/BOD theoretical
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
07-JAN-2005 (9)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 50 mg/l
**Degradation:** = 70 - 74 % after 30 day(s)
**Result:** other: well biodegradable

**Method:** other: RDA-Test according to Blok (AWU)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft 63-79% BSB30/BSBT ungenügend Restsauerstoff CSB= 1.97mg O2/mg AS BSBT=3.19mg O2/mg AS
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 74% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 70% with parameter % BSB/ThSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions

concerning this end point. A source of higher reliability is available.

28-SEP-2005 (10) (15) (16)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 50 mg/l
**Degradation:** = 73 - 82 % after 30 day(s)
**Result:** other: well biodegradable

**Method:** other: RDA-Test according to Blok (AWU)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parallel wurde eine Testreihe ohne Zwischenbelüftung geprüft
46-61% BSBT CSB= 1.97mg O2/mg AS BSBT=3.19mg O2/mg AS
**Source:** Henkel KGaA Duesseldorf
**Test condition:** 1: 50 mg/l referring to Chemical oxygen demand: 82% with parameter % BSB/ThSB
#2: 50 mg/l referring to Chemical oxygen demand: 73% with parameter % BSB/ThSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

28-SEP-2005 (11) (15) (17)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 43800 - 45300

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be

overestimates
**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.
21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty

alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (7)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** other: mortality
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male
**No. of Animals:** 20
**Vehicle:** other: 50% w/w in peanut oil at 40C
**Doses:** 10 g/kg
**Value:** > 10000 mg/kg bw

**Method:** other: contract laboratory protocol
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: One test animal died following dosing.
- Time of death: not reported
- Number of deaths at each dose: 1/10 at 10g/kg Epal 1618.

CLINICAL SIGNS: Loose stools were observed in the peanut oil controls on the first observation day. No signs were reported for the treated group. Both surviving treated rats and the solvent controls gained weight normally over the observation period.

NECROPSY FINDINGS: Assume unremarkable as no statement made.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: Males only tested.

**Source:** Carter et al. 1975
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley (CD)
- Source: not reported
- Weight at study initiation: 200-300 g
- Group size: 10M fasted
- Controls: 10M (solvent treated) fasted

ADMINISTRATION: Gavage
- Doses: 10 g/kg
- Doses per time period: single
- Volume administered or concentration: 50% in peanut oil, controls received peanut oil.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality, body weight and clinical signs were monitored. Survivors were sacrificed and autopsied.

**Test substance:** Tradename Epal 1618 linearity unstated (probably linear)

**Conclusion:** The rat oral LD50 for Epal 1618 was >10 g/kg. One test animal died but other than this there were no reported signs of

intoxication.

This value is also reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Study not well documented but appears to be carried out adequately.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (5) (22)

**Type:** LD50
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 20
**Vehicle:** other: 20% aqueous suspension prepared in 0.5% gum tragacanth
**Doses:** 2, 4, 5 and 10 g/kg,
**Value:** > 10000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died.

CLINICAL SIGNS: Not reported.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: Combined test group.
**Source:** Continental Oil Company 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Not reported
- Weight at study initiation: 200-245 g
- Group size: 5 (a group of 5 is used at each dose level but it is not clear how the sexes were distributed among the dose levels as the report states both were used). The rats were fasted.
- Controls: none

ADMINISTRATION: Gavage
- Doses: 2, 4, 5 and 10 g/kg (based on range finding test)
- Doses per time period: single
- Volume administered or concentration: 20% aqueous suspensioin in 0.5% gum tragacanth.
- Post dose observation period: 14 days
EXAMINATIONS: Mortality was recorded.
**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear
**Conclusion:** The rat oral LD50 for Alfol 1618 was >10g/kg.
**Reliability:** (2) valid with restrictions
Limited documentation but sufficient for assessment.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (6)

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white

**Sex:** no data
**No. of Animals:** 4
**Vehicle:** other: 20% aqueous suspension prepared in 0.5% gum tragacanth
**Doses:** 1, 2,5, 5 and 10 g/kg
**Value:** > 10000 mg/kg bw

**Method:** other: screening test.
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Alfol 1618 was administered to a single rabbit at each dose level. None of the animals died. The observation period was not reported but in a rat LD50 study referred to in the same report the observation period was 14 days. The results suggest that this material has an oral LD50 in rabbits of >10g/kg.
**Source:** Continental Oil Company, 1979
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear
**Reliability:** (2) valid with restrictions
Group size small, documentation limited but gives an indication of the level of toxicity.
04-AUG-2005 (6)

**Remark:** Unpublished data from Henkel KGaA Archive no TBD 720089

Rat oral LD50 carried out to an in-house protocol >10,000 mg/kg. No further details available.
**Test substance:** As prescribed in 1.1-1.4
**Reliability:** (4) not assignable
Secondary reference unpublished data.
29-OCT-2004 (22)

**Remark:** Unpublished data ex Henkel KGaA archive TBD 730111, 1973 and TBD 750143, 1975

The mouse oral LD50 was reported as >5000 mg/kg in 1973 and as >10,000 mg/kg in 1975. No further details available.
**Test substance:** As prescribed in 1.1-1.4
**Reliability:** (4) not assignable
Secondary reference unpublished data.
02-AUG-2005 (22)

## 5.1.2 Acute Inhalation Toxicity

**Type:** other: screening test with concentrated vapours
**Species:** rat
**Strain:** Sprague-Dawley
**Sex:** male/female
**No. of Animals:** 6
**Vehicle:** other: atmosphere of warmed concentrated vapours
**Doses:** dose level reported as concentrated vapours
**Exposure time:** 6 hour(s)

**Method:** other: in house protocol
**Year:** 1979

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All rats survived the exposure period and subsequent 14 day observation period.

CLINICAL SIGNS: Not reported.

NECROPSY FINDINGS: Unremarkable other than slight pulmonary congestion.

POTENTIAL TARGET ORGANS: Possible effect on the lungs.

SEX-SPECIFIC DIFFERENCES: None reported
**Source:** Continental Oil Company 1979
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear
**Conclusion:** This rat screening test indicates that a 6 hour inhalation exposure to the concentrated vapours of Alfol 1618 is not toxic. Gross necrospy revealed slight pulmonary congestion.
**Test condition:** TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: not reported
- Weight at study initiation: not reported
- Number of animals: 6 M+F
- Controls: none

ADMINISTRATION: 6 hour vapour exposure, whole body
- Type of exposure: vapour inhalation
- Concentrations: reported as a concentrated vapour only
- Particle size: vapour
- Type or preparation of particles: Vapour generated by by passing a stream of warm air over the material (at the melting point temperature).

EXAMINATIONS: Mortality was recorded during the 6 hour exposure and subsequent 14 day observation period. All animals were subjected to gross necropsy at the end of the observation period.
**Reliability:** (2) valid with restrictions
Study meets generally accepted scientific principles, some restrictions (limited reporting, vapour concentration not monitored) acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (6)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** no data
**No. of Animals:** 4
**Vehicle:** peanut oil
**Doses:** 8 g/kg as 50% in vehicle
**Value:** > 8000 mg/kg bw

**Method:** other: Contract laboratory protocol
**Year:** 1975
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure and observation period.

APPLICATION SITE: None reported.

CLINICAL SIGNS: None reported. The test animals showed a normal weight gain.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: Sex not specified.

**Source:** Carter et al. 1975
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported.
- Weight at study initiation: 2.3-3 kg
- Group size: 4 (sex unspecified
- Controls: no

ADMINISTRATION: 24 hour occluded exposure
- Area covered: trunk of animal
- Occlusion: plastic sleeve
- Vehicle: peanut oil
- Concentration in vehicle: 50%
- Doses: 8000 g/kg
- Removal of test substance: not reported

EXAMINATIONS: Mortality, behaviour and weight gain were observed over the 14 day observation period.

**Test substance:** Tradename Epal 1618 linearity unstated (probably linear)

**Conclusion:** The rabbit dermal LD50 (24 hour occluded) for Epal 1618 was >8000 mg/kg applied as a 50% solution in peanut oil. There were no deaths or reports of toxicity.

This value reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Study meets generally accepted scientific principles, some restrictions (limited reporting) acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (5) (22)

**Type:** other: screening test
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** no data
**No. of Animals:** 5
**Vehicle:** other: undiluted (heated to melting point)
**Doses:** 1, 2.5, 5, 7.5 and 10 g/kg
**Value:** > 10000 mg/kg bw

**Method:** other: screening test
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** All 5 animals survived. The MLD was found to be greater than

10,000 mg/kg bw.
**Source:** Continental Oil Company 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** One rabbit was exposed at each of 5 dose levels ranging from 1 to 10 g/kg. The treated area was covered with a plastic shield for an exposure period of 24 hours. The animals were then observed for 14 days.
**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear
**Reliability:** (2) valid with restrictions
Group size small, documentation limited but gives an indication of the level of toxicity.
04-AUG-2005 (6)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** other: New Zealand White rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** peanut oil
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24 + 72 hour scores intact skin 3 rabbits 0.5, 1 rabbit 1.0, 1 rabbit 1.5 (group mean 24+72 hour scores 0.7); abraded skin 2 rabbits 0.5, 2 rabbits 1.0, 1 rabbit 1.5 (group mean 24+72 hour score 0.8).
- Oedema: All scores 0.

REVERSIBILITY: By 72 hours post exposure erythema scores in 4 of the 5 surviving rabbits were 0, in the 5th rabbit the erythema score had reduced from 2 to 1.

OTHER EFFECTS: One animal died (no explanation given)
**Source:** Carter 1975
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported

- Weight at study initiation: Not reported
- Number of animals: 6 (5 assessed one died)
- Controls: No

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 50% in peanut oil
- Area of exposure: Not reported
- Occlusion: semi-occlusive
- Vehicle: Peanut oil
- Concentration in vehicle: 50%
- Exposure period: 24 hours
- Total volume applied: 0.5 ml
- Postexposure period: 72 hours
- Removal of test substance: Not reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours

**Test substance:** Tradename Epal 1618 linearity unstated (probably linear)
**Conclusion:** Following a 24 hour semi-occlusive exposure to rabbit skin Epal 1618 is classified as non-irritant based on either EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Limited documentation but sufficient for assessment.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (5) (23)

**Species:** other: New Zealand White Rabbit
**Exposure:** Occlusive
**Exposure Time:** 72 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: All scores 0
- Edema: All scores 0

OTHER EFFECTS: None reported.
**Source:** Continental Oil Company, 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: No

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: Not reported
- Occlusion: Occlusive

- Vehicle: None
- Concentration in vehicle:
- Exposure period: 24 hours
- Postexposure period: 72 hours
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours

**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear
**Conclusion:** Following a 24 hour occluded exposure to rabbit skin Alfol 1618 was non-irritating according to both EU and GHS criteria.
**Reliability:** (2) valid with restrictions
Limited documentation but sufficient for assessment.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (6)

**Remark:** Unpublished data ex Henkel KGaA as follows:

Archive 850044 Rabbit skin irritation test method unspecified. Result slightly irritating.

Archive TBD 870514 & 870515 Rabbit skin irritation test to OECD guide-line 404, Test substance Stenol 1618. Result Not irritating.

Archive RT920067 Rabbit skin irritation test to OECD guide-line 404. Result slightly irritating.

Archive TBD 700016 Hairless mouse, in house protocol. Results slightly irritating.

No further details available.
**Test substance:** As prescribed in 1.1-1.4 C16-18 alcohols CAS RN 67762-27-0
**Reliability:** (4) not assignable
Secondary reference unpublished data.
29-OCT-2004 (22)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand White Rabbit
**Concentration:** other: 20% suspension
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** no data
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no discernable eye irritation, all scores were 0 from 1 hour after instillation until 72 hours.
**Source:** Continental Oil Company 1979

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS:
- Strain: Rabbit
- Sex: New Zealand White
- Source: Not reported
- Age: Not reported
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: As a suspension (presume aqueous)
- Amount of substance instilled: 0.1 ml
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize
- Observation period: 72 hours
- Tool used to assess score: Fluorescein staining (2% aqueous solution)

**Test substance:** Tradename Alfol 1618 C16-18 alcohols 100% linear

**Conclusion:** Alfol 1618 was not an eye irritant according to EU or GHS criteria.

**Reliability:** (2) valid with restrictions
Limited documentation but sufficient for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (6)

**Species:** other: New Zealand White rabbits
**Concentration:** 50 %
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** other: peanut oil
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness, chemosis, discharge): scored together using the Draize calculation individual scores 4, 4, 2, 4, 0 at 24 hours and 0, 0, 0, 0, 2 at 48 hours.
- Overall score: Mean Draize score at 28 hours 2.8/110, at 48 hours 0.4/110.

DESCRIPTION OF LESIONS: Mild redness at 24 hours post instillation in 4 rabbits. Minimal redness in 1 rabbit at 48 hours.

REVERSIBILITY: All scores 0 by 72 hours and remaining 0 at day 7.

OTHER EFFECTS: One animal died, cause unreported. The remaining animals were scored.

**Source:** Carter 1975

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: not reported
- Source: not reported
- Age: not reported
- Number of animals: 6
- Controls: Untreated eye used as control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: prepared in vehicle at 40C. The material was a sticky waxy solid and could not be powdered and the melting point was too high to apply without causing heat damage.
- Amount of substance instilled: 0.1 ml
- Vehicle: peanut oil
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: not reported.

**Test substance:** Tradename Epal1618 Linearity unstated probably linear

**Conclusion:** Based on the Draize scores reported it is considered that Epal 1618 is not not an eye irritant according to either EU or GHS criteria.

**Reliability:** (2) valid with restrictions
Limited documentation but sufficient for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (5) (23)

**Remark:** Unpublished data ex Henkel KGaA as follows:

Archive no. TBD 850044 Rabbit eye irritation. Result slightly irritating.

Archive no. TBD 870514 and 870642 Rabbit eye irritation to OECD guide-line 405. Result slightly irritating. No other details available.

**Test substance:** As prescribed in 1.1-1.4 C16-18 alcohols CAS RN 67762-27-0

**Reliability:** (4) not assignable
Secondary reference unpublished data.

29-OCT-2004 (22)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction 5 % intracutaneous
**2nd:** Induction 5 % occlusive epicutaneous
**3rd:** Challenge 25 % open epicutaneous
**No. of Animals:** 40
**Vehicle:** other: 1st induction olive oil; 2nd induction vaseline; challenge vaseline or ethanol.
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: Magnusson & Kligman maximisation test

**Year:** 1969
**GLP:** no data
**Test substance:** other TS

**Result:** Study reported in summary individual animal data not provided but the test materials did not induce sensitisation reactions in the guinea pig.
**Source:** Gloxhuber, 1983
**Test condition:** TEST ANIMALS:
- Strain: guinea pig
- Sex: female
- Weight at study initiation: 400-500 g
- Number of animals: 20
- Controls: 20

ADMINISTRATION/EXPOSURE
- Study type: M&K maximization
- Preparation of test substance for induction: 5% intracutaneous in olive oil.
- Preparation of test substance for induction: 5% topical in vaseline.
- Concentrations used for induction: 25% topical in vaseline
- Concentration in Freuds Complete Adjuvant (FCA): 1:1
- Positive control: Not reported

**Test substance:** Several preparations were tested, hexadecanol, octadecanol, a mixture of C12/1C8 coco-alcohols, a mixture of C16/C18 tallow alcohols and Lanette 0, a trade product containing C16/C18 alcohols.
**Reliability:** (2) valid with restrictions
Comparative study to accepted method, limited reporting but acceptable for assessment.
04-AUG-2005 (8) (22)

**Remark:** Unpublished data ex Henkel KGaA. Archive TBD 780060.

This is a report of a Landsteiner sensitisation test in guinea pigs. Induction concentrations and frequency were 3 X 25% open epicutaneous and 7 X 10% open epicutaneous. The challenge concentration was 2 X 1% open epicutaneous.

The result was negative indicating that that the test substance is not a skin sensitiser.
**Test substance:** As prescribed in 1.1-1.4 C16-18 alcohols CAS RN 67762-27-0
**Reliability:** (4) not assignable
Secondary reference unpublished data.
30-OCT-2004 (22)

**Remark:** Unpublished data ex Henkel KGaA.
Achive R9601679 probably a Guideline study carried out at Huntingdon Research (Report 3/1988) to OECD guide-line 406. Guinea pig maximisation test. Result negative.

Archives TBD 770079 and 780103 report of Magnusson and Kligman guinea pig maximisation study, result negative.
**Test substance:** As prescribed in 1.1-1.4 C16-18 alcohols CAS RN 67762-27-0
**Reliability:** (4) not assignable
Secondary reference unpublished data.
30-OCT-2004 (22)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-acute
**Species:** other: albino rat **Sex:** male/female
**Strain:** other: Carworth CFN
**Route of administration:** inhalation
**Exposure period:** 8 hours
**Frequency of treatment:** daily, 5 days/week
**Post exposure period:** 14 days
**Doses:** 0.56 mg/l
**Control Group:** yes
**NOAEL:** < .56 mg/l
**LOAEL:** = .56 mg/l

**Method:** other: see text
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** All of the animals survived the exposure and observation periods. No gross signs of intoxication were noted during or prior to each exposure. Bodyweight loss, anorexia, generalized weakness and slight emaciation were recorded in some animals during the post-exposure period. Body weight loss generally corresponded with a reduced food intake and in the 4 animals affected ranged between 3.8 and 21.28%. Gross pathological examination revealed pulmonary lesions and discoloration of the kidneys. Histopathological examination (lung only examined) showed bronchopneumonic changes in 3 animals, changes in the other test animals were similar to those seen in the 2 untreated controls. These reactions could not be definitely attributed to the inhalation exposure of the animals to the test material according to the authors.
**Source:** Scientific Associates, Inc. 1968.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Weight at study initiation: 215 - 298 g
- Number of animals: 5M+5F treated, 1M+1F control

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: Daily, 8 hours/day for 10 days.
- Type of exposure: Whole body exposures to a mist.
- Post exposure period: 14 days
- Vehicle: Air
- Concentration in vehicle: Average over the 10 days 0.56 m/l (concentration varies between 0.16 and 0.89 mg/l, minimum desired concentration was 0.25 mg/l.
- Particle size: <= 5 microns
- Type or preparation of particles: The mist was generated using a DeVilbiss Nebuliser, flow rate 36 litres/minute.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: At 30 minutes intervals during exposure and daily during the post exposure period.
- Body weight: weekly
- Food consumption: weekly
- Water consumption: not measured

- Ophthalmoscopic examination: not done
- Haematology: not done
- Biochemistry: not done
- Urinalysis: not done

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: necropsy carried out
- Microscopic: lung tissues only

STATISTICAL METHODS: none

**Test substance:** C16-18 alcohols CAS RN 67762-27-0 (Alfol 1618)

**Conclusion:** This study is of limited value given the small numbers of animals, unexplained lack of control over exposure levels and limited evaluations carried out.

**Reliability:** (3) invalid
Significant methodological deficiencies see conclusion.

30-OCT-2004 (27)

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C16-18 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (1) valid without restriction
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (28) (29) (31)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C16-18 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (28) (29) (31)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (21) (28) (29) (31)

## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C16-18 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol) and

C22 (docosanol) and from the supporting substance C18 (octadecanol).
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (28) (29) (31)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C16-18 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (28) (29) (31)

### 5.8.3 Toxicity to Reproduction, Other Studies

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### 5.9 Specific Investigations

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### 5.10 Exposure Experience

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### 5.11 Additional Remarks

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(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

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(8) Gloxhuber, Ch. 1983 Bewertung der allergologishen Eigenshaften von cetyl- und stearylalkohol. Arztliche Kosmetologie 13:181-186

(9) Henkel KGaA, unpublished data (Registry No. 6603)

(10) Henkel KGaA, unpublished data, File 5, Page/Assay 27

(11) Henkel KGaA, unpublished data, File 5, Page/Assay 28

(12) Henkel KGaA, unpublished data, File 5, Page/Assay 29

(13) Henkel KGaA, unpublished data, File 5, Page/Assay 30

(14) Henkel KGaA, unpublished data, Final report

(15) Henkel KGaA, unpublished data, Final report 1986 2415

(16) Henkel KGaA, unpublished data, Protocol 1, Page/Assay 27

(17) Henkel KGaA, unpublished data, Protocol 1, Page/Assay 28

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(19) Henkel KGaA, unpublished data, Protocol 1, Page/Assay 30

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(23) IUCLID data sheet. 1995g. C16-18.

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(25) Morris, P.A., Filler, P.A., and Nielsen, A.M. 1991. Sturm test evaluation of Alfol 1618-CG alcohol, Alfol 12 alcohol, Alfonic 1618-87 alcohol ethoxylate, and ditallow dimethyl ammonium methyl sulfate quaternary amine. Vista Chemical Company research report No. 6911-34-5-91.

(26) Safety data sheet Henkel KgaA

(27) Scientific Associates, Inc. 1968. Inhalation toxicity tests of Alfol 1618-C in rats. S.A. Number 149726.

(28) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(29) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(30) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(31) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(32) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 67762-30-5 |
| **CAS No.** | 67762-30-5 |
| **EINECS Name** | Alcohols, C14-18 |
| **EC No.** | 267-009-1 |
| **TSCA Name** | Alcohols, C14-18 |

| | |
|---|---|
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |

| | |
|---|---|
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **29-DEC-2005** |
| **Number of Pages:** | **41** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

04-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. Dave Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, Texas
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CCHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C14-18 alcohols, CAS 67762-30-5 are 100% linear (or unstated).

The substance comprises >95% C14, 16 and 18. Components of even chain length, in the range C10-C20 are present.

Commercial products marketed under this CAS number fall into two types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A and Type B.

Type A products are 100% linear (or unstated). The substance comprises >=95% c16 and 18. Components of even chain length, in the range C12-C20 are present.

Type B products are 100% linear (or unstated). The substance comprises >95% C14, 16 and 18. Components of even chain length, in the range C10-C20 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C14-18 (CA INDEX NAME)
Alfol 1418DDB
Alfol 1620
Alfolt 1418DDB
C14-18 alcohols
C14-18-alkanols
C14-C18 alcs.
CO 1418
Harchemex
Sidopol

TA 1618E

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C14-18 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is

the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (4) (11) (15)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**-**

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.
The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some

Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (17)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C14-18 alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required

11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
17-OCT-2005 (1)

## 2.2 Boiling Point

**Value:**

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
**Reliability:** (2) valid with restrictions
06-JAN-2005 (1)

## 2.3 Density

**Type:** density
**Value:** = .79 - .83 at 80 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (10)

**Type:** density
**Value:** = .79 - .8 g/cm³ at 80 degree C

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (12)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000017 - .00009 hPa at 25 degree C

**Method:** other (calculated)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:

Type A: 0.000017 hPa
Type B: 0.00009 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** 6 - 7.2 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Result:** Type A: 6.7-7.2
Type B: 6.0-7.2
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
21-JUL-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .035 - .12 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.035 mg/l at a loading rate of 1000 mg/l
Type B: 0.12 mg/l at a loading rate of 1000 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** at 20 degree C
**Descr.:** not soluble

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (12)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 170 degree C
**Type:** open cup

**Method:** other: DIN ISO 2592

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
21-JUL-2005 (12)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (10)

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (10)

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (10)

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section

1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
13-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** Type A:

| | |
|---|---|
| TGD hydrophobics method: | Koc = 307000 - 839000 |
| TGD Non-hydrophobics method: | Koc = 30100 - 57400 |
| TGD Alcohols method: | Koc = 1240 - 2010 |
| SRC PCKOCWIN method: | Koc = 3790 - 12900 |

Type B:

| | |
|---|---|
| TGD hydrophobics method: | Koc = 96500 - 839000 |
| TGD Non-hydrophobics method: | Koc = 14300 - 57400 |
| TGD Alcohols method: | Koc = 710 - 2010 |
| SRC PCKOCWIN method: | Koc = 1110 - 12900 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by

section 1.1-1.4. All components are predicted to be readily biodegradable, though the ten-day window may not be met. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to both compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

**Type:** aerobic
**Inoculum:** other bacteria: aus ueberwiegend kommunalem Abwasser
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Degradation:** = 73 % after 28 day(s)

**Method:** other: BOD-Test for insoluble substances (BODIS). Closed
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Parameter: % BOD/COD
**Source:** Henkel KGaA Duesseldorf
**Test condition:** Testsubstanz einzige C-Quelle; kontinuierlich geschuettelt
**Test substance:** Kettenlaenge: C14 - C18
It is not possible to determine which compositional Type was tested

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original report has not been reviewed further because it was not available for review, due to change of business circumstances.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4.

05-OCT-2005 (6)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 33900 - 45300

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log

Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Result:** Type A: BCF predicted to be 43800 - 45300
Type B: BCF predicted to be 33900 - 45300

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A and B: >100 mg/l (i.e. predicted to be non-toxic at the limit of solubility)

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A and B: >100 mg/l (i.e. predicted to be non-toxic at the limit of solubility)

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For both compositional Types A and B, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The values obtained by prediction are:

Types A and B: Both predicted to be non-toxic at the limit of solubility.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (2)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine

oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (5)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** mouse
**Strain:** other: CF1
**Sex:** male
**No. of Animals:** 10
**Vehicle:** other: 25% suspension
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died.

CLINICAL SIGNS: No signs of toxicity.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: Males only tested.

**Source:** Henkel KGaA 1977
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: mouse (CF1)
- Source: no data
- Weight at study initiation: average body weight 25g
- Group size: 10M fasted
- Controls: No

ADMINISTRATION: Gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 25% suspension administered as in a constant volume of 20 ml/kg.
- Post dose observation period: 8 days

EXAMINATIONS: Mortality and clinical signs.

**Test substance:** C14-18 alcohols insufficient compositional information to ascribe a type.

**Conclusion:** Mouse oral LD50 >5000 mg/kg. There were no mortalities or signs of toxicity at this dose level.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

02-AUG-2005 (7)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12 (1-dodecanol), C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18, and C18 (octadecanol) alcohols in support of the statement that C14-18 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (13) (14) (16)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20) including data for C12 (1-dodecanol), C14 (1-tetradecanol), C16 (1-hexadecanol), C12-16 and C20 (eicosanol) alcohols which support the statement that C14-18 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (13) (16)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. Higher members of the sub-category of linear alcohols (C12 and above) have a skin irritation

potential in the range mild - essentially non-irritant, when applied undiluted for 4 - 24 hours. Alcohols with a carbon chain length >C18 were generally without a skin irritation response. Data are available for C12 (dodecanol), C14 (tetradecanol), C16 (hexadecanol), C16-18 and C18 (octadecanol) linear alcohols which support the conclusion that C14-18 alcohols are expected to be mildly irritating to the skin.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** C14-18 alcohols are expected to be mildly irritating to the skin.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (13) (14) (16)

## 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants while alcohols of chain length >C12 for C12 (dodecanol), C14-16, C16 (hexadecanol) and C18 (octadecanol) alcohols support the conclusion that C14-18 alcohol is expected to be essentially non-irritating to the eye

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** C14-18 alcohol is expected to be essentially non- irritating to the eye.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

29-DEC-2005 (13) (14) (16)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C12 (dodecanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C14-18 alcohols are not expected to be skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

05-DEC-2005 (13) (14) (16)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C14-18 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (13) (14) (16)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C14-18 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (13) (14) (16)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to

C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (8) (13) (14) (16)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C14-18 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol) and C22 (docosanol) and from the supporting substance C18 (octadecanol).

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (13) (14) (16)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of

linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C14-18 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (13) (14) (16)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

**Type:** other: comment on Iuclid 2000

**Remark:** In the existing Iuclid data base for this Cas# there are various entries however none related specifically to this Cas#.

30-OCT-2004 (9)

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(6) Henkel KGaA, unpublished data (Pruefnr. 6603).

(7) Henkel KGaA. 1977. Alcohols, C14-18: Evaluation of acute oral toxicity. Unpublished data, Report No. TBD 770019 and summary data 1999. (Study report 62)

(8) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(9) Iuclid 2000 European Commission - European Chemicals Bureau Alcohols C14-18 Cas# 67762-30-5

(10) IUCLID data sheet. 1995f. C14-18.

(11) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(12) Safety data sheet Henkel KgaA

(13) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(14) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(15) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(16) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(17) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 67762-41-8
**CAS No.** 67762-41-8
**EINECS Name** Alcohols, C10-16
**EC No.** 267-019-6
**TSCA Name** Alcohols, C10-16

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
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**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

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04-AUG-2005

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**Remark:** Industry Consortium
23-AUG-2005

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20-DEC-2005

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20-DEC-2005

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20-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

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20-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** OH 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C10-16 alcohols, CAS 67762-41-8 are 5-100% linear.

The substance comprises C10-16 alcohols. Components of even and odd chain length, in the range C8-C18 are present.

Commercial products marketed under this CAS number fall into four types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A, Type B, Type C and Type D.

Type A products are 100% linear. The substance comprises >80% C10, 12 and 14, <10% C16. Components of even chain length, in the range C8-C18 are present.

Type B products are 5-50% linear. The substance comprises >=95% C12 and 13. Components of even and odd chain length, in the range C11-C14 are present.

Type C products are 80-95% linear. The substance comprises >95% C12 and C13. Components of even and odd chain length, in the range C11-15 are present.

Type D products are 40-50% linear. The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C11-C16 are present.

17-OCT-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C10-16 (CA INDEX NAME)
Alc., C10-16
Alcs., C10-16

C10-16 alcohols
C10-16-alcs.
Lial 123
Lorol Special

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C10-16 alcohols.

Composition is described in section 1.1.1, General Substance Information.

17-OCT-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the

public domain:

USA: ca. >50 000 - 250 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >100 000 000 - 500 000 000 pounds.

21-DEC-2005 (4) (32) (54)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available
17-OCT-2005

**Use category:** 35 Lubricants and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available
17-OCT-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary

**Emission scenario document:** not available
17-OCT-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

-

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification NWG or 1 ID No. 71, 1482 and 656
17-OCT-2005 (57)

## 1.8.4 Major Accident Hazards

-

## 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

-

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C10-16 alcohols. There could also be exposure from private use (for consumer products).

17-OCT-2005

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

17-OCT-2005

## 2.1 Melting Point

**Value:** = 0 degree C

**Method:** other: ASTM E5327-84
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The freezing point was determined using Differential Scanning Calorimetry.
**Test substance:** This result was measured for a test substance of compositional Type B.
**Reliability:** (1) valid without restriction
GLP compliant study
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (45)

**Value:** = 18.5 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.IUCLID 2000 CD-ROM, and cannot be validated further. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** > 255 degree C at 1013 hPa

**Method:** Directive 92/69/EEC, A.2
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Reported value was measured at atmospheric pressure.

Tests at reduced pressures were also conducted.
**Result:** Under a reduced pressure of 13 hPa, the substance distilled between 144 - 147 and 140 - 143 deg C.
**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction
GLP-compliant, standard study.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (45)

**Value:** = 265 - 280 degree C at 1013 hPa
**Decomposition:** no

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
05-JAN-2005

**Value:**

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Value:** = .844 at 20 degree C

**Method:** Directive 92/69/EEC, A.3
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a test substance of compositional Type B.
**Reliability:** (1) valid without restriction
GLP-compliant, standard study.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (45)

**Type:** density
**Value:** = .831 g/cm³ at 20 degree C

**Remark:** The IUCLID 2000 robust summary gave the value as 831 but it is assumed that the actual value was 0.831.
**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005

**Value:** = .831 at 20 degree C

**Reliability:** (4) not assignable
21-OCT-2005 (55)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** It is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (53)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00053 - .0029 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.0029 value hPa
Type B: 0.00083 value hPa
Type C: 0.00082 value hPa
Type D: 0.00053 value hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (1)

**Value:** = .681 hPa at 25 degree C

**Method:** Directive 92/69/EEC, A.4
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The static method was used.
**Remark:** Reviewer's comment: The measured vapour pressure is much higher than would be expected from its measured boiling range and from the known vapour pressure of its components. This is a problem inherent to the method used (static method) because it reflects the total vapour pressure of the substance. Even traces of absorbed water, or very minor impurities, can have a big influence on the value measured by this method. Therefore, although the Reliability of the study is 1 - valid without restriction, the results do require the above additional interpretation.
**Result:** The report also derived a vapour pressure of 0.495 hPa at 20 degrees C.
**Test substance:** This result was measured for a test substance of compositional Type B.
**Reliability:** (1) valid without restriction
GLP-compliant, standard study.
11-OCT-2005 (45)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 6

**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (50)

**Partition Coeff.:** octanol-water
**log Pow:** = 4.8

**Method:** Directive 92/69/EEC, A.8
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (1) valid without restriction
GLP-compliant, standard study.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (45)

**log Pow:** = 4.6 - 6.4 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected

to significantly affect the predicte value. Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

**Result:** Type A: 4.6 - 6.0
Type B: 5.4 - 5.6
Type C: 5.4 - 5.5
Type D: 5.4 - 6.4

**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.

**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 2.4 mg/l at 25 degree C

**Method:** other
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (15)

**Solubility in:** Water
**Value:** = 2.9 mg/l at 20 degree C

**Method:** Directive 92/69/EEC, A.6
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Result is 2.9 +/- 0.8 mg/l.
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (1) valid without restriction
GLP-compliant, standard study.
**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (45)

**Solubility in:** Water
**Value:** = .67 - 7.1 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed,

validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 7.1 mg/l at a loading rate of 1000 mg/l
Type B: 1.1 mg/l at a loading rate of 1000 mg/l
Type C and D: 0.67 mg/l at a loading rate of 1000 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

13-SEP-2005 (1)

## 2.6.2 Surface Tension

**Value:** = 53.9 mN/m at 20 degree C
**Concentration:** 2.7 mg/l

**Method:** Directive 92/69/EEC, A.5
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** In pure water, the value is 71.6 mN/m. The surface tension stabilises at 53.9 mN/m.

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction
GLP-compliant, standard study.

11-OCT-2005 (45)

## 2.7 Flash Point

**Value:** > 110 degree C
**Type:** closed cup

**Method:** Directive 92/69/EEC, A.9
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction

11-OCT-2005 (45)

**Value:** = 126 degree C
**Type:** closed cup

**Method:** other
**GLP:** no

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (21)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of flashpoint. It is not possible to estimate with confidence what the flashpoint might be.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005

## 2.8 Auto Flammability

**Value:** = 242 degree C at 1017 hPa

**Method:** Directive 92/69/EEC, A.15
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (1) valid without restriction
11-OCT-2005 (45)

## 2.9 Flammability

**Year:** 1998
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Based on the structure, the substance would not be expected to produced flammable gases in contact with water.

The substance would not be expected to have pyrophoric properties.
**Reliability:** (2) valid with restrictions
Theoretical conclusions drawn as part of a high-reliability overview of physicochemical properties.
11-OCT-2005 (45)

## 2.10 Explosive Properties

**Result:** not explosive
**Test substance:** as prescribed by 1.1 - 1.4
**Reliability:** (1) valid without restriction
11-OCT-2005 (45)

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Type:** air
**Light source:** Sun light
**INDIRECT PHOTOLYSIS**
**Sensitizer:** OH
**Conc. of sens.:** 1000000
**Rate constant:** = .000000000013358 $cm^3$/(molecule * sec)
**Degradation:** = 50 % after 19.2 hour(s)

**Method:** OECD Guide-line draft "Photochemical Oxidative Degradation in the Atmosphere"
**Year:** 1990
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (55)

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint

21-JUL-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:** Type A:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 6330 - 307000 |
| TGD Non-hydrophobics method: | Koc = 2490 - 30100 |
| TGD Alcohols method: | Koc = 190 - 1240 |
| SRC PCKOCWIN method: | Koc = 90 - 3790 |

Type B:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 40100 |
| TGD Non-hydrophobics method: | Koc = 6420 - 7680 |
| TGD Alcohols method: | Koc = 390 - 450 |
| SRC PCKOCWIN method: | Koc = 330 - 600 |

Type C:
TGD Hydrophobics method: Koc = 27600 - 36600
TGD Non-hydrophobics method: Koc = 6420 - 7680
TGD Alcohols method: Koc = 390 - 450
SRC PCKOCWIN method: Koc = 330 - 600

Type D:
TGD Hydrophobics method: Koc = 27600 - 177000
TGD Non-hydrophobics method: Koc = 6420 - 23100
TGD Alcohols method: Koc = 390 - 1020
SRC PCKOCWIN method: Koc = 330 - 2050

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only for the upper limit of the range.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

28-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 12.8 mg/l related to Test substance
25.9 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 86 - 87 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:** 7 day(s) = 52 %
14 day(s) = 72 %
21 day(s) = 78 %
28 day(s) = 87 %
**Control Subst.:** other: Sodium acetate

**Method:** other: Directive 92/69/EEC, C.4-C and OECD Guide-line 301B
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The first value cited in the results section is for the 25.9 mg/l concentration and the second number is for the 12.8 mg/l concentration. The following validity criteria were fulfilled: 1) Parallel assays did not differ by more than 20% (2) the reference compound reached the pass level of 60% within 14 days, 3) the total inoculum blank CO2 production amounted to 24.2 mg CO2/l at the end of the test.
**Result:** Kinetic of control substance: 7 days = 51%
14 days = 70%
21 days = 77%
28 days = 87%
The substance degraded >60% over the test period and the 10-day windown criterion was met, therefore the substance is considered to be readily biodegradable.

**Test condition:** Inoculum concentration: 30 mg/l solid substance
Test volume: 1 litre
Temperature: 20 +/- 2 C
pH: 7.4 - 7.6
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (1) valid without restriction
GLP-compliant, standard study
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (44)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 35 mg/l related to Test substance
54 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 84 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:** 1 day(s) = 10 %
8 day(s) = 60 %
17 day(s) = 79 %
28 day(s) = 84 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: OECD Guide-line 301 F and ISO 9408
**Year:** 1993
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test was conducted with two samples at different concentrations (35 and 54 mg/l relating to Test substance). Biodegradation values reported are the mean of these two samples. The following validity criteria were met (1) Parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level of 60% by day 14, (3) O2 uptake in the inoculum blank was less than 60 mg/l over 28 days.
**Result:** Kinetic of control substance: 1 day = 40%
8 days = 80%
17 days = 93%
28 days = 85%
The substance degraded >60% over the test period and met the 10-day window criterion, therefore it is considered readily biodegradable.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
Guideline study conducted to GLP, but some experimental details not reported.
**Flag:** Critical study for SIDS endpoint
28-SEP-2005 (26)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 46 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 80 % after 28 day(s)
**Result:** readily biodegradable

**Kinetic:** 1 day(s) = 3 %
8 day(s) = 63 %
17 day(s) = 82 %
28 day(s) = 80 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: OECD 301F and ISO 9408
**Year:** 1993
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were met (1) Parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level of 60% by day 14, (3) O2 uptake in the inoculum blank was less than 60 mg/l over 28 days.
**Result:** Kinetic of control substance:
1 days = 40%
8 days = 60%
17 days = 93%
28 days = 87%
The substance degraded >60% over the test period and met the 10-day window criterion, therefore it is considered readily biodegradable.
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Guideline study conducted to GLP, but some experimental details not reported.
17-OCT-2005 (24)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 45 mg/l related to Test substance
**Contact time:** 37 day(s)
**Degradation:** = 91 % after 26 day(s)
**Result:** readily biodegradable
**Kinetic:** 2 day(s) = 11 %
8 day(s) = 62 %
15 day(s) = 81 %
26 day(s) = 92 %
37 day(s) = 92 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: OECD 301F and ISO 9408
**Year:** 1993
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were met (1) Parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level of 60% by day 14, (3) O2 uptake in the inoculum blank was less than 60 mg/l over 28 days.
**Result:** Kinetic of control substance: 2 days = 61%
8 days = 83%
15 days = 87%
26 days = 90%
37 days = 91%
The substance degraded >60% over the test period and met the 10-day window criterion, therefore it is considered readily

biodegradable.
**Test condition:** Inoculum concentration: not reported
Temperature: not reported
Test volume: 500 ml
pH: not reported
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Guideline study conducted to GLP, but some experimental details not reported.
05-OCT-2005 (25)

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to all compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other
**Year:** 1974
**GLP:** no data
**Year:**
**Method:** The tests were conducted in accordance with the 'Standard Dilution Method' at 20 C for a period of 5 days. This method is described in APHA 'Standard Methods' Nr.219 and was formerly included in the ASTM Standards under Nr. D2329-68. For practical reasons the official Netherlands method NEN 3255 5.4 was used. The only difference in the NEN procedure compared with the others is that consumption of oxygen as a result of nitrification is prevented by the addition of allylthiourea. The test solutions were seeded with 10 ml/l of the effluent of a biological sanitary waste treatment plant.
**Remark:** BOD measurements were expressed as weight of oxygen per weight of chemical (g/g) and, if composition of the product was known, as a percentage of the theoretical oxygen demand,

ThOD (%).
**Result:** BOD 5 = 0.72 - 1.59 g/g
%ThOD = 51%
>50% degradation, therefore was grouped into good degradability class
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
17-OCT-2005 (16)
**Method:**

**C O D**

**Method:** other
**Year:** 1974
**GLP:** no data
**COD:** = 2.81 mg/g substance
**Method:** In the COD test (ASTM D 1252-67) the oxidizable material present in waste water is oxidised by a standard potassium dichromate solution in 50% sulfuric acid. The mixture is refluxed at about 145 C for two hours. The excess dichromate is then titrated and the COD calculated.
**Result:** The COD was found to be 2.81 g/g.
90% oxidation to water and carbon dioxide was also calculated.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
17-OCT-2005 (17)

## 3.7 Bioaccumulation

**BCF:** = 1500 - 45300

**Method:** other: calculated (based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Result:** Type A: BCF predicted to be 1530 - 45300
Type B: BCF predicted to be 4500 - 9600

Type C: BCF predicted to be 7200 - 9600
Type D: BCF predicted to be 4500 - 42600

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 4 - 10
**Limit Test:** no

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Five fingerlings, weighing 1 to 1.4 g, were placed in each 10 litre aquarium. Test concentrations ranged from 1 to 10 mg/l. The test solutions were maintained at 15-16 C and pH 8.3-8.4
**Remark:** Cloudiness was observed at the 10 mg/L concentration. At higher concentrations the test material precipitated out of solution.

The solubility of C12, the lowest carbon chain length in the compound is approximately 2 mg/l.

The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.
**Result:** RESULTS: EXPOSED
LC50 = 4-10 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Shell Toxicology Laboratory. 1978a. The acute toxicity of DOBANOL-23 to rainbow trout (Salmo gairdneri). GRR-TLGR.0161.78.
**Test condition:** TEST ORGANISMS
Strain: Salmo gairdneri
Supplier: Itchen Valley Trout Farm, Alresford, hampshire, UK
Weight: 1-1.4 g
Feeding: Not reported
Pretreatment: Not reported
Feeding during test: Not reported
Control group: 1 solvent control group (5 fish)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle, solvent: 900 mg/l
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Mains water
Aeration: Continuous gentle aeration
Alkalinity: Not reported
Hardness: 230 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 1, 3, 4, 6, 8, 10 mg/l

Renewal of test solution: none
Exposure vessel type: 10 l glass aquaria
Number of replicates: 1
Fish per replicate: 5
Test temperature: 15-16 C
Dissolved oxygen: 9.5-9.8 mg/l
pH mean: 8.3-8.4
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: mortality
SAMPLING: Not reported
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
19-OCT-2005 (49)

**Type:** static
**Species:** Carassius auratus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** > 2.4
**Limit Test:** no

**Method:** other: ASTM Method D 1345. Test for Evaluating Acute Toxicity of Industrial Waste Water to Fresh-Water Fishes.
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The experiments were performed in aquaria with 25 L of test solution and 6 or 10 goldfish.
**Result:** The test substance was found to be non-toxic at the saturated aqueous solution of 2.4 mg/l.
**Source:** Bridie et al. 1973.
**Test condition:** Temperature was 20 C; pH was 7.8; dissolved oxygen was 9-10 mg/L; hardness was not reported. Fish averaged 6.2 cm length and 3.3 grams.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) containing greater detail are available.
20-OCT-2005 (15)

**Type:** semistatic
**Species:** other: juvenile turbot (Scophthalmus maximus)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 10
**Limit Test:** no

**Method:** other
**Year:** 1991
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 18 mg/l was the highest test concentration employed in the

test due to the limited solubility of the test substance in water and having regard to the amount of auxiliary solvent permitted in the test. At levels in excess of 18 mg/l most of the test substance was seen to form a waxy solid on the surface of the water.

Test was carried out in synthetic sea water (Synthetica) at 32% S.

The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.

**Source:** Huntingdon Life Sciences Ltd. 1991c.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
This test was conducted with a marine species.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (23)

**Type:** semistatic
**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = 10
**LL50 :** = 15
**LL100 :** = 32
**Limit Test:** no

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
NOEL = 10 mg/l
LL50 = 15 mg/l
Based on loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0
The measured values in fresh test medium were much lower than the loading rates and during the test they decreased further. This can be explained by solubility limits of the components of the test substance and the biodegradation that may have occurred during the water accommodated fraction (WAF) preparation and during exposure. The toxicity is described on the basis of loading rates.
**Source:** TNO 2000a.
**Test condition:** TEST ORGANISMS
Strain: Brachydanio rerio
Supplier: Atlanta (Marconiweg 56, Hellevoetsluis)
Weight: 0.08 g
Feeding: Fed until 24 h prior to test
Pretreatment: Not reported
Feeding during test: None
Control group: 1 control group (Dilution water as control media)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Not reported

Concentration of vehicle/solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTION
not reported
DILUTION WATER
Source: Prepared by addition of several salts to ground water from a locality near Linschoten (the Netherlands)
Aeration: Slight aeration
Alkalinity: Not reported
Hardness: 197 mg/l (CaCO3)
Conductance: Not reported
TEST SYSTEM
Loading rates: 10, 18, 32, 56, and 100 mg/l
Renewal of test solution: daily
Exposure vessel type: 2 l glass beaker
Number of replicates: 1
Fish per replicate: 10
Test temperature: 25 C
Dissolved oxygen: 6.3 - 8.2 mg O2/l
pH mean: 8.0-8.3
Adjustment of pH: none
Intensity of irradiation: not reported
Photoperiod: 16 h light/8 h dark regime
TEST PARAMETER: mortality
SAMPLING: Animals monitored and dead ones removed at 3, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: 0 and 24 h
Measured values were much lower than the loading rates and during the test they decreased to values of 0.6% of the loading rates.

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (46)

**Unit:** mg/l **Analytical monitoring:** no

**LC50:** = .52 - 2.6 calculated

**Method:** other

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.

**Result:** The range of results given above reflects variable composition

between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.52 mg/l
Type B: 0.62 mg/l
Type C: 0.61 mg/l
Type D: 2.6 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

21-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** = .23
**EL50 :** = .28
**Limit Test:** no

**Method:** other: Based on OECD Guideline 202
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of two commercial products to D. magna was determined in sealed 72 h toxicity tests. The test solutions were prepared as WAFs and were renewed at approximately 24 hour intervals. The test material was directly added to the WAF preparation vessels using ethanol as a carrier (0.1 mL/L). The vessels were then stirred at approximately 100 rpm for a period of approximately 24 hours, before running off the WAFs for use as the test media.
**Remark:** The quoted EL50 values are the loading rate resulting in 50% immobilization.
**Result:** RESULTS: EXPOSED
EL50 = 0.28 mg/l (Type C)
EL50 = 0.23 mg/l (Type B)
Based on loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Palmer and Cann 2000a.
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24 hours old
Feeding: Algae daily (Chlorella vulgaris)
Pretreatment: None
Feeding during test: Not reported
Control group: Two control flasks containing reconstituted water only and a further two flasks to which ethanol had been added at 0.1 ml/L
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Ethanol

Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS:
Considered stable
DILUTION WATER
Source: Reconstituted fresh water
Aeration: Not reported
Alkalinity: Not reported
Hardness: 172-176 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Loading rates: 0.03, 0.1, 0.3, 1.0, and 3.0 mg/l
Renewal of test solution: Every 24 hours
Exposure vessel type: 150 ml glass flasks
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: 6.8-8.4 mg/l (Type C), 7.2-8.4 mg/l (Type B)
pH mean: 7.6-8.3 (Type C), 8.2-8.9 (Type B)
Adjustment of pH: Not reported
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Every 24 hours. The mean decrease in levels of the components of the Type C test substance during the two 24h periods of use was 68% (range 54 to 83%). The mean decrease in levels of the components of the Type B test substance during the two 24h periods of use was 53% (range 25 to 81%).

**Test substance:** This results were measured for commercial products of compositional Types B and C.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
20-OCT-2005 (33)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** < 1
**Limit Test:** yes

**Method:** OECD Guide-line 202
**Year:** 2001
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test was carried out with Water accommodated fractions (WAFs), at a loading rate of 1 mg/l, which had been filtered prior to use.

The total measured concentration of the water accommodated fraction of the test substance in test media was 0.41 and 0.29 mg/l at 0 and 24 hours respectively. The mean decrease in levels of the components during the first 24 h period of use was 29%. The data for the 48 hour exposure is not included due to a mix-up between the control and 1 mg/l loading rate.
**Source:** Palmer and Cann 2001a.
**Test substance:** This result was measured for a commercial product of compositional Type C.

**Reliability:** (2) valid with restrictions
Not key study: Other studies with same reliability score and showing greater toxicity are available.
20-OCT-2005 (34)

**Type:** semistatic
**Species:** Crangon crangon (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** > 10
**Limit Test:** yes

**Method:**
**Year:** 1991
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 10 mg/l was the highest test concentration that could be prepared due to the limited solubility of the test substance in water and with regard to the amount of auxiliary solvent permitted in the test.
At levels in excess of 10 mg/l most of the test substance was seen to form a waxy solid on the surface of the water.
Test was carried out in synthetic sea water (Synthetica) at 32% S.
**Source:** Huntingdon Life Sciences Ltd 1991b.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and showing greater toxicity are available
17-OCT-2005 (22)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** = 2.8
**Limit Test:** no

**Method:** OECD Guide-line 202
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
EL0 = 0.32 mg/l
EL50 = 2.8 mg/l
EL100 = 10 mg/l
Based on loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** TNO 2000b.
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: TNO
Age: Not reported
Feeding: Algae (Chlorella) and yeast
Pretreatment: None
Feeding during test: None

Control group: 4 replicates exposed to dilution water only
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTIONS:
Not reported
DILUTION WATER
Source: Ground water
Aeration: None
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0, 0.32, 1.0, 3.2, 10, and 32 mg/l
Renewal of test solution: None
Exposure vessel type: 600 ml glass beakers
Number of replicates: 4
Invertebrate per replicate: 5
Test temperature: 20 C
Dissolved oxygen: 7.0 mg O2/l
pH mean: 8.0-8.2
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 16 hour light - 8 hour dark regime
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION: Every 24 hours
The measured values were much lower than the loading rates and during the test they decreased further.

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (47)

**Unit:** mg/l **Analytical monitoring:** no

**EC50:** = .21 - .49 calculated

**Method:** other

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described

by the present CAS number.

The values obtained by prediction are:
Type A: 0.31 mg/l
Type B: 0.49 mg/l
Type C: 0.48 mg/l
Type D: 0.21 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** =
**NOEL :** = .03
**EL50 :** = .1 - .3
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 1984
**GLP:** yes

**Method:** The acute toxicities of two commercial products to R. subcapitata were determined in 72 h growth inhibition toxicity tests. Algal inocula were exposed to test solutions which were not renewed during the test. The quoted EL50 values are the loading rate resulting in 50% inhibition.

**Result:** RESULTS: EXPOSED
TYPE C:
EbL50 = 0.03 - 0.1 mg/l (Area under growth curve)
ErL50 = 0.1 - 0.3 mg/l (Average specific growth rate)
TYPE B:
EbL50 = 0.1 - 0.3 mg/l (Area under growth curve)
ErL50 = 0.1 - 0.3 mg/l (Average specific growth rate)
Based on loading rates
For the Type C and Type B test substances, the ranges for the EbL50 and ErL50 were 0.1 to 0.3 mg/L respectively with one exception; the EbL50 for Type C was in the range 0.03 to 0.1 mg/L.

**Source:** Palmer and Cann 2000a.

**Test condition:** TEST ORGANISMS
Strain: Raphidocelis subcapitata
Supplier: Institute of Freshwater Ecology, Windermere
Pretreatment: Not reported
Controls: 2 sets of controls (7 flasks in each), one containing ethanol at 0.1 ml/L
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Ethanol
Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS
Considered stable

DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, and 1 mg/l
Renewal of test solution: None
Exposure vessel type: 287 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 5000 cells/ml
Test temperature: 21.1-24.1
Dissolved oxygen: Not reported
pH mean: 7.2-9.3
Adjustment of pH: None
Intensity of irradiation: 5020-5353 lux
Photoperiod: Under constant illumination
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION:
At the start and end of the test. Concentration of the Type C test substance in test media decreased by 11-90% over 72 hours. Test media concentrations for the Type B test substance decreased by 27-72% over the
72 hour test period.

**Test substance:** This results were measured for commercial products of compositional Types B and C.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (33)

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: biomass and growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EbL50 :** < 1
**ErL50 :** < 1
**Limit Test:** yes

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2001
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test was carried out with Water accommodated fractions (WAFs), at a loading rate of 1 mg/l, which had been filtered prior to use. The total concentrations of the water accommodated fraction of test substance in test media were 0.39 and 0.07 mg/l at 0 and 72 hours respectively. The mean decrease in levels of the components during the period of use was 82%.

**Source:** Palmer and Cann 2001a.

**Test substance:** This result was measured for a commercial product of compositional Type C.

**Reliability:** (1) valid without restriction
Not key study: Other studies with same reliability score and showing greater toxicity are available.

17-OCT-2005 (34)

**Species:** other algae: Pseudokirchneriella subcapitata
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = .6
**ErL50 :** = 2.2
**EbL50 :** = 1
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2003
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** WAFs were prepared by loading test medium with the respective amount of the test item. After stirring the contents were left to settle for 24h. The WAFs were filtered prior to use through a non polar filter (0.2 um Millex FG, 50 mm, Millipore).
**Result:** RESULTS: EXPOSED
Growth rate
NOEL = 0.6 mg/l
LOEL = 1.2 mg/l
ErL10 = 0.5 mg/l
ErL50 = 2.2 mg/l
Biomass
EbL10 = 0.6 mg/l
EbL50 = 1.0 mg/l
Based on loading rates
**Source:** Wenzel 2003.
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and showing greater toxicity are available
17-OCT-2005 (58)

**Species:** Selenastrum capricornutum (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** = .058
**EbL50 :** = .23
**ErL50 :** = .44

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 1984
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
NOEL = 0.058 mg/l
EbL50 = 0.23 mg/l (Area under growth curve)
ErL50 = 0.44 mg/l (Growth rate)
Based on loading rates
**Source:** TNO 2001.
**Test condition:** TEST ORGANISMS
Strain: Selenastrum capricornutum

Supplier: American Type Cell Culture, Maryland, USA
Pretreatment: Not reported
Controls: 4 controls (2 without tert-butyl alcohol and 2 containing 100 ul tert-butyl alcohol)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water Accommodated Fractions
Vehicle, solvent: TBA (tert-butyl alcohol)
Concentration of vehicle, solvent: 1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Loading rates: 0.033, 0.058, 0.10, 0.19, 0.33, 0.58, and 1.0 mg/l
Exposure vessel type: Flask
Number of replicates: 2
Initial cell concentration: 8000 cells/ml
Test temperature: Not reported
Dissolved oxygen: Not reported
pH mean: 8.3 - 8.8
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION:
At the beginning and end of test
The measured concentrations were found to be between 63 and 94% of the nominal concentrations at the start of the test and between 30 and 52% at the end of the test

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

19-OCT-2005 (48)

**EC10:** calculated

**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although

it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

For Types A and D, for which estimation of algal toxicity is required, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A and D: both 0.1 - 1.0 mg/l
For Types B and C, reliable measurements are available and so these have not been estimated.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.
**Source:** de Wolf and Parkerton 1999.
**Reliability:** (2) valid with restrictions
30-OCT-2003 (19)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | Wistar |
| **Sex:** | male/female |
| **No. of Animals:** | 6 |
| **Vehicle:** | other: undiluted |
| **Doses:** | 2000 mg/kg |
| **Value:** | > 2000 mg/kg bw |
| **Method:** | OECD Guide-line 423 |
| **Year:** | 1998 |
| **GLP:** | yes |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: None of the test animals died during the study.<br><br>CLINICAL SIGNS: Diarrhoea was observed in 1 male and 2 females within 4 hours of dosing. 2 females showed piloerection within 1 hour of dosing while the remaining female showed sluggishness and piloerection within 1 and 4 hours and hunching and blepharospasm within 1 hour. During the remainder of the 14 day observation period none of the animals showed any clinical signs. All animals gained weight normally during the study.<br><br>NECROPSY FINDINGS: Unremarkable<br><br>POTENTIAL TARGET ORGANS: None identified<br><br>SEX-SPECIFIC DIFFERENCES: No difference in mortality females showed more clinical signs immediately after dosing but all normal within 24 hours. |
| **Source:** | Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Rat (Wistar Crl:(W1) WU BR<br>- Source: Charles River, Wiga, Germany<br>- Age: 5-6 weeks<br>- Weight at study initiation: mean bodyweight males 215g, females 151g<br>- Group size: 3M+3F<br>- Controls: no<br><br>ADMINISTRATION: gavage, animals fasted overnight<br>- Doses: 2000 mg/kg<br>- Doses per time period: single (the 3 females were dosed first followed after 4 hours by the males)<br>- Volume administered or concentration: undiluted<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Clinical signs were observed at 1 and 4 hours |

after dosing and daily throughout the observation period. Body weights were recorded immmediately prior to dosing and at days 3, 7 and 14. All survivors were necropsied at the end of the observation period.

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** The rat oral LD50 for Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A) is >2000 mg/kg. There was no target organ toxicity. Transient signs of intoxication occurred within a few hours of dosing and included diarrhoea, piloerection and lethargy. Findings at gross necropsy were unremarkable.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

18-OCT-2005 (36)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: undiluted
**Doses:** 10 g/kg
**Value:** > 10000 mg/kg bw

**Method:** other: standard in house protocol
**Year:** 1978
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died during the study.

CLINICAL SIGNS: Diarrhoea, piloerection, and epistaxis was observed within 7 hours post-dosing. Greasy, soiled fur was present on days 2 and 3.

NECROPSY FINDINGS: Necropsy results were not reported.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None

**Source:** Cassidy, 1978c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall) breeding unit, Sittingbourne, UK
- Age: 6 weeks approx.
- Weight at study initiation: not reported
- Group size: 4M+4F
- Controls: no

ADMINISTRATION: gavage, animals fasted
- Doses: 1000 and 2000 mg/kg
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Deaths and clinical signs of intoxication were observed over the 14 day observation period. All decedents and

survivors received a gross post mortem examination.
**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C
**Conclusion:** The rat oral LD50 for Dobanol 23 was >10 g/kg. No target organ was identified. Transient diarrhoea, piloerection and epistaxis was observed on the day of dosing.

This study is reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (18) (28)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1990
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No deaths occurred during the test or observation period.

CLINICAL SIGNS: No alterations in clinical observations and no loss of body weight were observed.

NECROPSY FINDINGS: None reported

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None
**Source:** Biolab SGS 1990a
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan-Correzzana, Milan, Italy
- Age: young adults
- Weight at study initiation: 200 g +- 20 g
- Group size: 5M+5F
- Controls: 5M+5F

ADMINISTRATION: Gavage, animals fasted
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical examination several times during the first day after dosing then daily. Survivors are weighed at the end of the observation period and subjected to gross necropsy.
**Test substance:** Tradename Alchem 123 C10-16 alcohols Type C
**Conclusion:** The rat oral LD50 for Alchem 123 is > 5 g/kg. There were no signs of intoxication at this dose level.
**Reliability:** (2) valid with restrictions

Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (10)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 40
**Vehicle:** water
**Doses:** 2900, 3460, 4160 and 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No deaths occurred during the test or observation period.

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: None reported

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan-Correzzana, Milan, Italy
- Age: young adults
- Weight at study initiation: 200 g
- Group size: 5M+5F
- Controls: no

ADMINISTRATION: Gavage, animals fasted
- Doses: 2900, 3460, 4160 and 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 2 ml/100g
- Post dose observation period: 14 days

EXAMINATIONS: Clinical examination several times during the first day after dosing then daily. Survivors are weighed at the end of the observation period and subjected to gross necropsy.
**Test substance:** Tradename Lial 123 C10-16 alcohols Type B
**Conclusion:** The rat oral LD50 for Lial 123 is > 5 g/kg.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions such as limited reporting of results.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (5)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 20
**Vehicle:** other: undiluted
**Doses:** 5000 mg/kg

**Value:** > 5000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No deaths occurred during the test or observation period.

CLINICAL SIGNS: No clinical signs of intoxication.

NECROPSY FINDINGS: None reported

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan-Correzzana, Milan, Italy
- Age: young adults
- Weight at study initiation: 200 g +- 20g
- Group size: 5M+5F
- Controls: 5M+5F

ADMINISTRATION: Gavage, animals fasted
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: Undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical examination several times during the first day after dosing then daily. Survivors are weighed at the end of the observation period and subjected to gross necropsy.

**Test substance:** Tradename Isalchem 123 C10-16 alcohols Type B
**Conclusion:** The rat oral LD50 for Isalchem 123 is >5000 mg/kg, there were no clinical signs of toxicity.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions such as limited reporting of results.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (13)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Inhalation: Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C8 (1-octanol), C8-10, C10 (1-decanol), C12 (1-dodecanol), C12-16 (Type A), C14 (tetradecanol), C16 (hexadecanol), C16-18 and C20 (eicosanol) alcohols in support of the statement that C10-16 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration..
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially

saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion that the LC50 is expected to be greater than the substantially saturated vapour concentration are based are either comparable to guideline studies or publications with sufficient detail for assessment.
12-SEP-2005 (51) (56)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: undiliuted
**Doses:** 1000 and 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** other: Noakes and Sanderson, 1969
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: day 6 and day 8
- Number of deaths at each dose:

1000 mg/kg F 0/4, M 0/4
2000 mg/kg F 0/4, M 2/4

Combined LD50 >2000 mg/kg. Male LD50 ca 2000 mg/kg

APPLICATION SITE: reactions at the application site were not reported.

CLINICAL SIGNS: Rats showed hyper-reactivity to stimuli at both dose levels on day 3. Male rats at the 2000 mg/kg level also became aggressive at this time.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: Male rats appeared more sensitive.
**Source:** Cassidy, 1978c
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall), Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F
- Controls: No

ADMINISTRATION: 24 hour occluded dermal application
- Area covered: not reported applied to shorn dorsolumbar skin.
- Occlusion: aluminium foil and waterproof plaster.
- Vehicle: undiluted

- Total volume applied: ca 2 ml/kg
- Doses: 1000 and 2000 mg/kg
- Removal of test substance: washed with tepid dilute detergent solution.

EXAMINATIONS: Mortality and clinical signs during the 14 day observation period.

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C

**Conclusion:** The rat dermal LD50 for Dobanol 23 (24 hour occluded) was >2000 mg/kg (M+F). Signs of intoxication were hyperactivity in both sexes and agression in males.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (18) (28)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** OECD Guide-line 402 "Acute dermal Toxicity"
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure period and subsequent 14 day observation period.

APPLICATION SITE: No signs of irritation were observed.

CLINICAL SIGNS: None observed. All animals gained in body weight over the 14 day observation period following a slight dip in weight at day 3.

NECROPSY FINDINGS: Unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: RAt (Wistar)
- Source: Charles River, Wiga, Germany
- Age: 7-8 weeks
- Weight at study initiation:
- Group size: 5M+5F
- Controls: none

ADMINISTRATION: 24 hour occlusive exposure to rat skin
- Area covered: at least 4cm x 5cm
- Occlusion: plastic foil attached by adhesive tape and wrapped with impervious material.
- Vehicle: Undiluted

- Total volume applied: 2.5 ml/kg
- Doses: 2000 mg/kg
- Removal of test substance: Any residue removed with water.

EXAMINATIONS: Clinical signs were observed within 1 and 4 hours of administration and daily thereafter. Body weights were recorded on the day of dosing and days 3, 7 and 14 of the observation period. Dermal reactions were scored (Draize) immediately after exposure and on days 3, 7 and 14 of the observation period. All survivors were necropsied.

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** The rat dermal LD50 (24 hour occluded) was >2000 mg/kg. There was no irritation at the application site and no clinical signs of toxicity. Necropsy findings were unremarkable.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

18-OCT-2005 (37)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** other: New Zealand white albino rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: individual mean 24+48+72 hour scores were 2 in all animals.
- Oedema: individual mean 24+48+72 hour scores were 1.3 in all animals.

REVERSIBILITY: The skin of all animals appeared normal at 7 days.

OTHER EFFECTS: Slight scaliness was observed at 48 and 72 hours after patch removal.

**Source:** Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Male
- Source: Broekman Institute, Someren, The Netherlands
- Age: Young adults
- Weight at study initiation: 2.042 - 2.28 kg
- Number of animals: 3
- Controls: No reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2.5x2.5 cm
- Occlusion: semi-occluded
- Vehicle: none
- Total volume applied: 0.5 ml
- Exposure time: 4 hours
- Postexposure period: 7 days
- Removal of test substance: Using tissue moistened with water

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours then at 7 days

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** Following a 4 hour semi-occlusive exposure to rabbit skin this C10-16 alcohol was found to be a skin irritant according to EU criteria (group mean 24+48+72 hour score 2 for erythema). According to GHS criteria this alcohol would be considered as a mild irritant (Category 3) as all individual scores for erythema were between 1.5 and 2.3.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

18-OCT-2005 (38)

**Species:** other: New Zealand White rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1984
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 1.7, 2, 2, 1.7, 1 and 1.7 (Group mean 1.63)
- Oedema: Individual 24+48+72 hour scores 2, 1.7, 1.7, 1.7, 1, 1.7 (Group mean 1.56)

REVERSIBILITY: The effects did not fully reverse over the time course of the study although they did regress. Group mean scores at 5 days were 1.3 for erythema and 1.1 for oedema. At 7 days the scores were 1.0 for erythema and 0.5 for oedema.
OTHER EFFECTS: None reported

**Source:** Biolab SGS 1984a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Lial 123 C10-16 alcohols Type B

**Conclusion:** Following a 4 hour occluded exposure to rabbit skin Lial was not a skin irritant according to EU criteria (group mean 24+48+72 hour scores for erythema and oedema <2). Using GHS criteria Lial 123 is classifiable as a mild (slight) irritant (category 3) as individual 24+48+72 hour scores erythema and oedema were all between 1.5 and 2.3.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (14)

**Species:** rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** no data
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1991
**GLP:** yes
**Test substance:** other TS: Alcohols C10-16, CAS RN 67762-41-8 (Lial 123)

**Result:** AVERAGE SCORE:
- Erythema: Group mean 24+48+72 hours score 1.5
- Oedema: Group mean 24+48+72 hours score 1.3
Individual scores were not available.

REVERSIBILITY: There was some evidence of reversibility although there remained evidence of irritation at the end of the 7 days exposure period. Group mean erythema score for day 7 was 1. Group mean oedema scores on days 5 and 7 were 0.5.

OTHER EFFECTS: None reported
**Source:** Biolab SGS, 1991b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Area of exposure: 6x6 cm
- Occlusion: Semi-occluded
- Vehicle: None reported assume undiluted
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.c

**Test substance:** Tradename Lial 123 C10-16 alcohols Type B
**Conclusion:** Following a 4 hour semi-occlusive exposure to rabbit skin LIAL 123 was not irritating according to EU criteria but would be considered a mild irritant using GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (8)

**Species:** rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** no data
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1991
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE:
- Erythema: Group mean 24+48+72 hour score 0.3.
- Edema: Group mean 24+48+72 hour score 0.2.
Individual scores were not available.

REVERSIBILITY: All scores were 0 on days 5 and 7.

OTHER EFFECTS: None reported.
**Source:** Biolab SGS, 1991c
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbits

- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Area of exposure: 6x6 cm
- Occlusion: Semi-occluded
- Vehicle: None reported assume undiluted
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Alchem 123 C10-16 alcohols Type C

**Conclusion:** Following a 4 hour semi-occlusive exposure to rabbit skin Alchem 123 was not irritating to the skin by either EU or GHS criteria.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (9)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1991
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE:
- Erythema: Individual mean 24+48+72 hour scores: 3 rabbits scored 0, the remaining 3 scored 0.7. Group mean 24+48+72 hours score 0.3.
- Edema: Individual mean 24+48+72 hour scores: 2 rabbits scored 1, the remaining 4 scored 0.7. Group mean 24+48+72 hours score 0.7.

REVERSIBILITY: At 72 hours the only evidence of irritation was oedema in 2/6 rabbits. All scores were 0 by day 5.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS, 1991a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits

- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Isalchem 123 C10-16 alcohols Type B
**Conclusion:** Following a 4 hour occlusive exposure to rabbit skin Isalchem 123 was classified as non irritating to skin using both EU and GHS classification systems.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
18-OCT-2005 (11)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**PDII:** 3.25
**Result:** irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE:
- Erythema: Individual mean 24+72 hour scores intact and abraded skin 1.75, 1.75, 2.25 (Group mean 24+72 hour score 1.9)
- Oedema: Individual mean 24+72 hour scores intact and abraded skin 1.5, 1.5, 1 (Group mean 24+72 hour score 1.35)

Primary Irritation Index 3.25.

REVERSIBILITY: The effects persisted for the 7 day observation period with a slight decrease in erythema but an increase in oedema. Group mean scores at 7 days were 1.5 for erythema and 2 for oedema.

OTHER EFFECTS: At 7 days the skin at all (intact and abraded) test sites was ridged, thickened and flaky.

**Source:** Cassidy 1978c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: female
- Source: Shell Toxicology Breeding Laboratory, Sittingbourne, UK
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2x2 cm
- Occlusion: occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 24 hours to intact and abraded skin.
- Postexposure period: 7 days
- Removal of test substance: Washed with warm dilute detergent solution.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours and at 7 days.

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C

**Conclusion:** Following a 24 hour occlusive exposure to rabbit skin Dobanol 23 is considered as an irritant when classified by EU and GHS criteria due to the persistence of the irritant response.

This result is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (18) (28) (29)

**Species:** rabbit
**Concentration:** other
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** water
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 92/69/EEC, B.4
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: 0
- Edema: 0

REVERSIBILITY: Not applicable as no irritant response

OTHER EFFECTS: None

**Test condition:** TEST ORGANISMS: Rabbit New Zealand White
- Source: Charles River Italia S.p.A
- Age: 3 months
- Weight at study initiation: 2.7-3.2 kg
- Number of animals: 3
- Controls: No

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 0.5g of test material was ground to a fine powder and moistened with 1 ml water
- Area of exposure: 6 cm2
- Exposure time: 3 minutes and 1 hour (1 animal); 4 hours all 3 animals.
- Occlusion: occlusive
- Postexposure period: 72 hours
- Removal of test substance: Residual material removed with water at the end of each exposure period.

EXAMINATIONS
- Scoring system: As for guideline
- Examination time points: Immediately and 72 hours after the 3 minute and 1 hour exposure period and at 1, 24, 48 and 72 hurs after the 4 hour exposure period.

**Test substance:** Tradename Isalchem 123A C10-16 alcohols Type B
**Conclusion:** Isalchem 123/A is not irritating to the skin of rabbits when assessed using EU and GHS criteria.
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
02-JAN-2006 (30)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 92/69/EEC, B.4
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: 0
- Edema: 0

REVERSIBILITY: Not applicable as no response

OTHER EFFECTS: None

**Test condition:** TEST ORGANISMS: Rabbit New Zealand White
- Source: Charles River Italia S.p.A
- Age: 3 months
- Weight at study initiation: 2.7-3.2 kg
- Number of animals: 3
- Controls: No

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 0.5g undiluted

- Area of exposure: 6 cm2
- Exposure time: 3 minutes and 1 hour (1 animal); 4 hours all 3 animals.
- Occlusion: occlusive
- Postexposure period: 72 hours
- Removal of test substance: Residual material removed with water at the end of each exposure period.

EXAMINATIONS
- Scoring system: As for guideline
- Examination time points: Immediately and 72 hours after the 3 minute and 1 hour exposure period and at 1, 24, 48 and 72 hurs after the 4 hour exposure period.

**Test substance:** Tradename Isalchem 123/AD C10-16 alcohols Type B
**Conclusion:** Isalchem 123/AD is not irritating to the skin of rabbits when assessed using EU or GHS criteria.
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
02-JAN-2006 (31)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand white albino rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: An amount of 0.1 ml of test material was instilled in the conjunctival sac of the right eye. The upper and lower lids were then held together for 1 second. The left eye was untreated and served as the control.
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0
- Conjunctivae (Chemosis): 0

DESCRIPTION OF LESIONS: At 1 hour after treatment, slight redness of the conjunctivae (grade 1 vessels definitely injected) was observed in all animals. At 24, 48, and 72 hours, no signs of eye irritation were observed in any of the 3 animals.

REVERSIBILITY: Fully reversible in the 72 hour observation period.

OTHER EFFECTS: None reported
**Source:** Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male

- Source: Broekmamn Institute, Someren, the Netherlands
- Age: Young adults
- Weight at study initiation: 1.87 - 2.132 kg
- Number of animals: 3
- Controls: untreated eyes

ADMINISTRATION/EXPOSURE
- Preparation of test substance: applied undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 72 hours

IN VITRO TEST SYSTEM
- Cell type: Chicken enucleated eye test used as an initial screen.
- Test conditions: not reported

EXAMINATIONS
- Scoring system: As in guideline
- Observation period: 72 hours
- Tool used to assess score: not reported

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A) is not an eye irritant according to EU or GHS criteria.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

18-OCT-2005 (39)

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1985
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual scores 2, 2, 1, 1, 1.3, 1,7 (group mean score 1.47)
- Conjunctivae (Chemosis): 1, 1, 1, 1.3, 1.3, 1.7 (group mean score 1.2)

REVERSIBILITY: Conjunctival redness and chemosis persisted in all test animals to 7 days, all individual scores for both parameters were 1.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS undated (a)
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Lial 123 C10-16 alcohols Type B

**Conclusion:** Lial 123 is not an eye irritant according to EU or GHS criteria taking into account the scores for 6 test animals. Although conjunctival redness and chemosis persisted through the 7 day observation period it was reduced at this time period and there was no involvement of the cornea and iris.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (12)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0 at all time points including 1 hour
- Iris: 0 at all time points including 1 hour
- Conjunctivae (Redness): individual scores 5 rabbits 0, 1 rabbit 0.7. (group mean score 0.11)
- Conjunctivae (Chemosis): individual scores 0, 0, 0.3, 0.3, 0.3, 0.7 (group mean score 0.28)

REVERSIBILITY: All scores were 0 at day 7.

OTHER EFFECTS: The mean scores for conjunctival redness and chemosis at 1 hour were 1.67.

**Source:** Biolab SGS 1991f
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White

- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Alchem 123 C10-16 alcohols Type C
**Conclusion:** Alchem 123 is not an eye irritant by either EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (6)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores 5 rabbits 0, 1 rabbit scored 1 (grou mean score 0.167)
- Iris: individual scores 5 rabbits 0, 1 rabbit scored 1 (group mean score 0.167)
- Conjunctivae (Redness): 5 rabbits 1, 1 rabbit scored 1.67 (group mean score 1.1)
- Conjunctivae (Chemosis): 5 rabbits 1, 1 rabbit scored 1.67 (group mean score 1.1)

REVERSIBILITY: Effects on the cornea and iris observed in one animal persisted through day 3 but had completely reversed by day 7. Conjunctival redness and chemosis was still evident in all eyes (grade 1) at day 7 (group mean 7 days scores were 1).

OTHER EFFECTS: The maximum effect was observed at 1 hour post instillation and was reduced in all animals at subsequent observation times.
**Source:** Biolab SGS 1991g
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: rabbit

- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Isalchem 123 C10-16 alcohols Type B

**Conclusion:** Isalchem 123 is not an eye irritant according to EU or GHS criteria taking into account the scores for 6 test animals. Although conjunctival redness and chemosis persisted through the 7 day observation period it was reduced at this time period and there was minimal involvement of the cornea and iris which was confined to one test animal.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (7)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .2 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0
- Conjunctivae (Chemosis): 0

DESCRIPTION OF LESIONS: Minimal conjunctival redness was observed at 1-2 hours after instillation (group mean score 0.5). Individual scores were not reported.

REVERSIBILITY: Complete

**Source:** Cassidy, 1978c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White

- Sex: not reported
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit.
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.2 ml
- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: not reported
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: Not reported

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C

**Conclusion:** Dobanol 23 was not an eye irritant according to EU or GHS criteria.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

20-JUL-2005 (18) (28) (29)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction .05 % intracutaneous
**2nd:** Induction 50 % occlusive epicutaneous
**3rd:** Challenge 25 % occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: corn oil
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: M&K guinea pig maximization test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: No details given.

RESULTS OF TEST
- Sensitization reaction: Response 0/20 treated, 0/10 control, result negative.
- Clinical signs: None in test or controls.
- Rechallenge: Not carried out.

**Source:** Cassidy, 1978c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: P-strain
- Sex: male & female
- Source: Shell Toxicology Lab (Tunstall) breeding unit.

- Age/weight: Not reported
- Number of animals: 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: Maximization (M&K)
- Preparation of test substance for induction: In corn oil
- Preparation of test substance for challenge: In corn oil
- Induction schedule: Intradermal injection followed one week later by topical application (48 hours occlusive).
- Concentrations used for induction: 0.05% intradermal, 50% topical.
- Concentration in Freuds Complete Adjuvant (FCA): no data
- Challenge schedule: 2 weeks after topical induction, 24 hour topical challenge.
- Concentrations used for challenge: 25% in corn oil.
- Rechallenge: No
- Positive control: Not reported

EXAMINATIONS
- Grading system: 4 point scale -ve, trace, +ve, ++ve
- Pilot study: Initial irritation screen, no details given.

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C

**Conclusion:** Dobanol 23 is not a skin sensitiser when tested according to the Magnusson & Kligman maximization procedure.

Study reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

05-DEC-2005 (18) (28)

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction 30 % intracutaneous
**2nd:** Induction 100 % occlusive epicutaneous
**3rd:** Challenge 100 % occlusive epicutaneous
**No. of Animals:** 10
**Vehicle:** physiol. saline
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** OECD Guide-line 406 "Skin Sensitization"
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: Intradermal - no irritation at test sites with 10 or 30% solutions in saline. The undiluted material caused abscesses, necrosis and incrustation. Topical - no irritation at either 30 or 100%.

RESULTS OF TEST
- Sensitization reaction: All scores 0 in test and control groups. Test 0/10, control 0/5.
- Clinical signs: Moderate erythema in treated and controls receiving FCA/saline, and controls receiving FCA/vehicle (grade 2). Intense erythema and swelling with necrosis and incrustation in test animals with FCA.
- Rechallenge: Not required

**Source:** Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: guinea pigs
- Strain: Dunkin Hartley albino
- Sex: male
- Source: Charles River, Germany
- Age: 4 weeks
- Weight at study initiation: 213-262g
- Number of animals: 10
- Controls: 5

ADMINISTRATION/EXPOSURE
- Study type: Ajduvant, M&K maximization
- Preparation of test substance for induction: intradermal in saline.
- Preparation of test substance for induction: Topical undiluted
- Induction schedule: Intradermal injection of test material in saline or saline+FCA. Topical application (48 hr occlusive) 1 week later. Test site pretreated with 10% SLS.
- Concentrations used for induction: 30%
- Concentration in Freuds Complete Adjuvant (FCA): 30%
- Challenge schedule: 14 days after induction application, topical application (24 hour occlusive).
- Concentrations used for challenge: Undiluted
- Rechallenge: No
- Positive control: Response of the test strain carried out with formalin at approximately 6 month intervals. Appropriate responses were obtained. Results were reported.

EXAMINATIONS
- Grading system: Intradermal Magnusson, Topical Draize.
- Pilot study: Intradermal injections in 2 animals at concentrations of 3, 10, 30 and 100%. Topical application in 2 animals at 30 and 100%.

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A) is not a skin sensitiser when tested using the guinea pig maximization procedure.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

30-DEC-2005 (40)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-acute
**Species:** rat **Sex:** male/female
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 28 days
**Frequency of treatment:** 7 days/ week
**Post exposure period:** none
**Doses:** 100, 300, and 1000 mg/kg bw
**Control Group:** yes, concurrent vehicle
**NOAEL:** = 300 mg/kg bw
**LOAEL:** = 1000 mg/kg bw

**Method:** OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"

**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL 300 mg/kg/day, LOAEL: 1000 mg/kg/day.
ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0. 100, 300 and 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: one high dose male died on day 27 (attributed to mis-dosing, confirmed by histopathological examination)

- Clinical signs: At the top dose most males (80%) & all females showed thinly haired areas of skin (probably hair nibbling). 3/5 top dose males showed weakness, thin appearance & respiratory disorders, one of these died on day 27. Top dose animals in particular showed some resistance to dosing. A few rats regurgitated the test material immediately after dosing.

- Body weight gain: Top dose males showed a reduction in mean body weights which reached statistical significance in the first and last weeks of the study ($p<0.05$). On day 27 the control body mean weight was 269 g while the mean for top dose males was 232 g.

- Food intake: Both food intake [control 17.3 g/rat/day; 1000 mg/kg/day 14.4 g/rat/day] and food conversion efficiency [control mean 0.23 g/g; top dose 0.17 g/g, the value for week 4 was -0.01] were reduced in top dose males.

- Clinical chemistry: Significant increases in high dose females for plasma ALP [control mean 101; test 150 U/l $p<0.05$], ALAT [control mean 27 U/l; test 39 $p<0.05$] and cholesterol [control mean 1.73; test 2.21 mmol/l $p<0.01$]. Increased albumin/globulin ratio in high dose males [control mean ratio 1.05, treated 0.88 $p<0.05$). Other parameters no significant differences.

- Haematology:
1000 mg/kg females: thrombocyte count significantly reduced [control 1185 10E9/l; treated 1066 $p<0.01$]; monocytes (absolute no) decreased [control 0 10E9/l; treated 0.04 $p<0.05$].
300 mg/kg males: MCH significantly reduced [control 1.34 fmol; test 1.26 $p<0.05$].
No other statistically significant changes.

- Organ weights: Dose related statistically significant increase in relative kidney wt in mid and top dose males [controls 6.80 g/kg bw, 100 mg/kg/day 7.15; 300 mg/kg/day 7.31 ($p<0.05$); 1000 mg/kg/day 7.80 ($p<0.01$). Absolute kidney weights showed no significant change from controls. There were no other significant changes in absolute or relative organ weights.

- Gross pathology: Pathologic changes in two high dose males (hydrothorax & spotted lungs in the animal which died) and a grossly abnormal thoracic cavity filled with fibrin in another male were associated with the dosing procedure.

- Histopathology: Histopathological changes in the rat which died were associated with mis-dosing of the test material and not considered treatment related. Histopathological changes in the 2 clinically affected top dose males were pericarditis in both animals, one male also exhibited, myocarditis and myositis. These changes were attributed to the administration procedure. There were no other treatment related histopathological changes.

**Source:** Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 5 weeks
- Weight at study initiation: males 144.2 -171.6 g (mean 159.3g); females 114.4 - 134.8 g (mean 124.7g)
- Number of animals: 5M+5F per treatment and control group.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 28 days
- Type of exposure: oral gavage
- Post exposure period: None
- Vehicle: Corn oil
- Concentration in vehicle: Adjusted to give a constant dosing volume.
- Total volume applied: 5 ml/kg
- Doses: 0, 100, 300 and 1000 mg/kg/day

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily, all abnormalities, signs of ill health and reactions to treatment were recorded.
- Mortality: Twice daily except weekends and holidays
- Body weight: Recorded on days 0,4,11, 14, 18, 21, 25, 27 and 28 (scheduled autopsy)
- Food consumption: Weekly (expressed as g/animal/day)
- Water consumption: Not recorded
- Ophthalmoscopic examination: Not carried out.
- Haematology: At day 28, Hb, PCV, RBC, total WBC, differential WBC, prothrombin time, thrombocyte count.
- Biochemistry: At day 28 plasma ALP, ASAT, ALAT, GGT, total protein, albumin , albumin/globulin ratio, rean, creatinine, fasting glucose, bilirubin, cholesterol, triglycerides, phospholipids, Ca, Na, Cl, inorganic phosphate. Animals fasted overnight prior to blood sampling.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full necropsy performed. Due to some difficulties during dosing it was decided to remove, examine and sample the oesophagus from all animals. However these samples were not processed for histopathological examination.
- Organ weights: adrenals, brain, kidneys, liver, spleen, testes
- Microscopic: Adrenals, heart, kidneys, liver, spleen, testes and gross lesions from all control and high dose animals.

STATISTICAL METHODS:
Body weights: one -way analysis of covariance (covariate body wt day 0) followed by Dunnetts multiple comparision tests
Food consumption: no statistics
Haematological parameters: one way analysis of covariance (ANOVA) followed by Dunnetts multiple comparision tests. For differential WBC Kruskal-Wallis non-parametric ANOVA followed

by Mann-Whitney U-tests.
Histopathology: Fischers exact probability test.

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)

**Conclusion:** At 300 and 1000 mg/kg/day there was an increase in relative kidney weights in males. Changes in clinical chemical parameters in top dose females were indicative of an effect on the liver. There were no accompanying histopathological changes in the liver or kidney. There were no changes in clinical chemical parameters indicative of an adverse effect on the kidney. The increase in kidney weight is therefore not considered a toxicologically significant effect. The decreased albumin/gobulin ratio in top dose males is of questionable biological significance given that total protein and albumin was comparable in all groups. The NOEL was 100 mg/kg/day. The NOAEL is considered to be 300 mg/kg/day.

**Reliability:** (1) valid without restriction
Guideline study

**Flag:** Critical study for SIDS endpoint

02-JAN-2006 (43)

**Type:** Sub-acute
**Species:** rat **Sex:** male
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 14 days
**Frequency of treatment:** daily
**Post exposure period:** no
**Doses:** 1 mmol/kg/day
**Control Group:** yes, concurrent vehicle

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** In vivo studies: There were no effects on relative testes weight, relative liver weight showed a slight* significant increase with 3,5,7-trimethyl hexanol. The postive control DEHP showed a clearly significant increase** in relative liver weight. There were no significant changes in testes weight relative to controls. Histopathological examination of the liver revealed no treatment related changes. Only the positive control DEHP showed any peroxisome proliferation or effects on cholesterol or triglycerides catalase was unaffected by treatment.
In vitro levels of palmitoyl CoA oxidase were increased only in the positive control group (MEHP).

**Source:** Rhodes et al, 1984
Hayes Consultancy Service Bromley, Kent

**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce hepatomegaly, peroxisome proliferation or hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any indication of testicular atrophy.

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol 300 as a vehicle and the test compounds a common dose level (on a molar basis) of 1 mmol/kg/day for 14

days. At the end of this period liver and testes weights were recorded. The liver was removed and samples taken for light and electron microscopy. The remaining liver was homogenised and prepared for assay of total catalase and CN-insensitive palmitoyl CoA oxidation. In vitro hepatocyte cultures were also prepared and the same compounds assessed for effects on CN-insensitive palmitoyl CoA oxidase activity after 72 hours incubation.

Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day

**Test substance:** Trade name Synprol C13-15 C10-16 alcohols Type D

Various alkanols were tested as follows:

Branched alcohols
2-ethyl hexanol C8
Iso-octanol C8
3,5,7-trimethylhexanol C9
Iso-nonanol C9
Iso-decanol C10
Tridecanol C13

Mixed branched & straight chain
Alphanol C7-9
Synprol C13-15 Cas RN 67762-41-8

Straight chain
Alfol C6-10 (Alfol 610) C6-10 (even) CAS RN 64365-05-5
Linevol C7-9 (Linevol 79) (even & odd) CAS RN 68603-15-6 (85% linear).

**Conclusion:** None of the alkanols investigated at dose levels of 1 mMol/kg showed any evidence of peroxisome proliferation, hepatomegaly, hepatomegaly, or hypolipidaemia. Testes weights were also unaffected by treatment.

**Reliability:** (2) valid with restrictions
Comparative research publicaton, study well documented, meets generally accepted scientific principles, acceptable for assessment.

20-JUL-2005 (35)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames Test)
**System of testing:** Salmonella typrhimurium strains TA98, 100, 1535, 1537

and 1538; Escherichia coli strains WP2 and WP2 uvrA
**Concentration:** 0, 0.2, 2, 20, 200 (or 500 E. coli) and 2000 ug/plate
**Cytotoxic Concentration:** >2000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 471
**Year:** 1980
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: There was no increase in reverse mutation rate in any of the test organisms. Appropriate responses were obtained with positive controls.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: >2000 ug/plate (highest dose level tested).

**Source:** Dean and Brooks 1980
Hayes Consultancy Service Bromley, Kent

**Test condition:** METHOD Ames test - similar to OECD 471, the top dose level of 2000 ug/plate was not cytotoxic.

SYSTEM OF TESTING
- Species/cell type: Salmonella typrhimurium strains TA98, 100, 1535, 1537 and 1538; Escherichia coli strains WP2 and WP2 uvrA
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0.2, 2, 20, 200 (or 500 for E.coli strains) and 2000 ug/plate
- Number of replicates: Duplicates
- Application: Vehicle DMSO
- Positive and negative control groups and treatment: Positive controls benzo[a]pyrene, sodium azide or nitroquinoline-n-oxide all at 20ug/plate
- Incubation time: 48 hours at 37C

CRITERIA FOR EVALUATING RESULTS: When expressed as a ratio (reverse mutation rate) a reproducible increase 2.5 times controls was considered positive.

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C
**Conclusion:** The C12-13 alcohol Dobanol 23 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium or E. coli in the presence or absence of metabolic activation at dose levels up to 2000 ug/plate. There was no evidence of cytotoxicity at any dose level.

Reported in Iuclid 2000

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (20) (28)

**Type:** Mitotic recombination in Saccharomyces cerevisiae
**System of testing:** Saccharomyces cerevisiae JD1
**Concentration:** 0.01, 0.1, 0.5, 1 and 5 mg/ml
**Cytotoxic Concentration:** >5 mg/ml
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: Saccharomyces gene conversion assay
**Year:** 1980
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No consistent increase in mitotic gene conversion at either the histidine or tryptophan locus.

PRECIPITATION CONCENTRATION: None reported.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: Not cytotoxic at any dose level tested.

**Source:** Dean & Brooks, 1980
Hayes Consultancy Service Bromley, Kent

**Test condition:** METHOD: Similar to OECD 481 but incubation periods were shorter and the test being negative was not repeated with stationary cells.

SYSTEM OF TESTING
- Species/cell type: Saccharomyces cerevisiae JD1 (growing cells)
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0.01, 0.1, 0.5, 1 and 5 mg/ml
- Number of replicates: Duplicates
- Application: Liquid suspension assay. Vehicle DMSO
- Deficiences/Proficiences: Histidine and tryptophan deficient
- Positive and negative control groups and treatment: Positive controls nitroquinoline-n-oxide 0.001 - 0.0001 mg/ml (-S9) and cyclophosphamide 10 mg/ml (+9).
- Incubation time: 1 hour prior to plating without S9 at room temperature, 1 or 4 hours with S9 at 37C. Plates were then incubated for 3 days at 30C.

CRITERIA FOR EVALUATING RESULTS: Reproducible values (conversion ratio) of greater than twice the control value indicates a postive resonse

**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C

**Conclusion:** The C12-13 alcohol Dobanol 23 did not increase the mitotic gene conversion rate in Saccharomyces cerevisiae in the presence or absence of metabolic acitivation. There was no evidence of cytotoxicity at any dose level.

Study reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (20) (28)

**Type:** Cytogenetic assay
**System of testing:** Rat liver cell cultures
**Concentration:** 0, 1.25, 2.5, 5 ug/ml
**Cytotoxic Concentration:** 10 ug/ml inhibited cell growth by 50%
**Metabolic activation:** without
**Result:** negative

**Method:** other: cytogenetic assay
**Year:** 1980
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
There was no increase in frequency in chromosome or chromatid aberrations compared to controls.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION: 10ug/ml which inhibited cell growth by 50%.
**Source:** Dean and Brooks 1980.

Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Rat liver cells (RL1)
- Metabolic activation system: inherent
- No. of metaphases analyzed: 100 per dose level

ADMINISTRATION:
- Dosing: 0, 1.25, 2.5 or 5 ug/ml based on initial cytotoxicity screen.
- Number of replicates: triplicate
- Application: Slide culture
- Positive and negative control groups and treatment: Positive control 7,12-dimethylbenzanthracene.
- Incubation time: 24 hours

CRITERIA FOR EVALUATING RESULTS: Assessment of incidence of different types of chromosome/chromatid aberrations.
**Test substance:** Tradename Dobanol 23 C10-16 alcohols Type C
**Conclusion:** The C12-13 alcohol Dobanol 23 did not increase the incidence of chromosome or chromatid aberrations in rat liver cells in culture at dose levels up to 5 ug/ml.

Study reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
20-JUL-2005 (20) (28)

**Type:** Bacterial reverse mutation assay
**System of testing:** Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537
**Concentration:** 62, 185, 556, 1667 and 5000 ug/plate; 2nd assay: 6, 18, 56, 167 and 500 ug/plate
**Cytotoxic Concentration:** 500 ug/plate

**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: The was no increase in reverse mutation rate in either of the assays carried out. An appropriate response was obtained in both negative and positive control groups.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: 500 ug/plate and above caused a marked decrease in the the mean number of revertant colonies.

**Source:** Hayes Consultancy Service Bromley, Kent
**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and a liver fraction of Aroclor 1254
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9, Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 1st assay: 62, 185, 556, 1667 and 5000 ug/plate; 2nd assay: 6, 18, 56, 167 and 500 ug/plate.
- Number of replicates: Triplicate, two independent assays carried out.
- Application: Plate incorporation assay, vehicle DMSO.
- Positive and negative control groups and treatment: Positive controls: (with S9) sodium azide 1 ug/plate; 9-aminoacridine 80 ug/plate; 2-nitrofluorene 2ug/plate; (without S9) 2-aminoanthracene 2 ug/plate, benzo[a]pyrene 4 ug/plate. Negative vehicle control DMSO.
- Incubation time: 72 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A reproducible two fold or greater increase in the mean number of revertant colonies above background or a demonstrable concentration based effect indicates a positive result. No statistical analysis is performed.

**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)
**Conclusion:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. There was marked cytotoxicity at dose levels of 500 ug/plate and above.
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
18-OCT-2005 (41)

**Type:** Cytogenetic assay
**System of testing:** Chinese hamster ovary cells (CHO K-1 line)
**Concentration:** Test 1: 0.1 - 500 ug/ml; Test 2: with S9 1 -50 ug/ml, without S9 0.5 - 20 ug/ml
**Cytotoxic Concentration:** +S9 40 ug/ml; -S9 15 ug/ml
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 473
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS: - With and without metabolic activation: There were no statistically significant increase in total numbers of chromosome aberrations at any dose level tested, the positive and negative controls showed an appropriate response. There was no increase in the incidence of polyploids or endoreduplicates.

PRECIPITATION CONCENTRATION: 125 ug/ml.

MITOTIC INDEX: The mitotic index was measured on 1000 cells and was always >40% of control levels and usually >50% for the dose levels which were scored for chromosome aberrations.

CYTOTOXIC CONCENTRATION:
- With metabolic activation: >= 40 ug/ml
- Without metabolic activation: >= 15 ug/ml

STATISTICAL RESULTS: Fischers exact probability test (two-sided) did not indicate any significant difference between test and control groups.

**Source:** TNO, 1998h
Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Chinese hamster ovary cells (CHO K-1 line)
- Metabolic activation system: Rat liver S9, Arochlor 1254 induced.
- No. of metaphases analyzed: 100 per culture

ADMINISTRATION:
- Dosing: Test 1: 0.1, 0.5, 1, 2.5, 5, 10, 20, 30, 50, 100, 125, 250, 500 ug/ml. Test 2: -S9 1, 2.5, 5, 7.5, 10, 15 and 20 ug/ml; +S9 1, 5, 10, 20, 30, 40 and 50 ug/ml.
- Number of replicates: Duplicates
- Application: 50 mg/ml in DMSO which produced a clear solution.
- Positive and negative control groups and treatment: Negative control DMSO, positive controls +S9 cyclophosphamide 3.75 ug/ml; -S9 mitomycin C 0.025 ug/ml
- Incubation time: Test 1: +S9 3 hours, -S9 18 hours, fixation time 18 hours. Test 2: +S9 3 hours with either 18 or 32 hours fixaton time; -S9 18 or 32 hours with 18 or 32 hours fixation time respectively.

CRITERIA FOR EVALUATING RESULTS: The test is considered positive if the aberration frequency of at least one concentration is significantly above concurrent control

frequencies.
**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)
**Conclusion:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A) did not increase the incidence of chromosome aberrations in Chinese hamster ovary cells at dose levels up to cytotoxic concentrations in the presence or absence of metabolic activation.
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
18-OCT-2005 (42)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5-C24-34) are negative. These include negative studies [Ames and chromosome aberrations] for C10-16 alcohols (types B and C)

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of systemic toxicity is based are either guideline or comparable studies or publications with sufficient detail for assessment.
12-SEP-2005 (27) (51) (52) (56)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Type:** other: Repeat dose study with histopathology of reproductive organs.
**Species:** rat
**Strain:** Wistar
**Route of administration:** gavage
**Exposure Period:** 28 days
**Frequency of treatment:** 7 days/week
**Duration of test:** 28 days
**Doses:** 100, 300, and 1000 mg/kg bw
**Control Group:** yes
**NOAEL Parental:** = 300 mg/kg bw

**Method:** other: OECD 407
**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were no adverse effects on the male reproductive organs as evidenced by lack of effect on relative testes weight and histopathological examination of the testes. Ovaries were not weighed and histopathological examination was not carried out. NOAEL for effects on the testes 1000 mg/kg/day (highest dose level tested).
**Source:** Hayes Consultancy Service Bromley, Kent
**Test condition:** The test material was applied to male and female Wistar rats (5 animals/sex/dose) via oral gavage in corn oil for 28 consecutive days (dosing volume: 5 ml/kg). The stability and homogeneity of the test material in the vehicle was checked via chemical analysis. Examinations included clinical signs, body weight, food consumption/food efficiency, haematology, clinical chemistry, gross necropsy and histopathological examination of several tissues. Histopathological examination was performed on the adrenals, heart, kidneys, liver, spleen, and testes.
**Test substance:** Safol(TM) 23 Alcohol C10-16 alcohols Type B (also known as Compound 33A)
**Reliability:** (1) valid without restriction
Guideline study
**Flag:** Critical study for SIDS endpoint
18-OCT-2005 (43)

**Type:** other: Comparative study including measurement of testes weight.
**Species:** rat
**Sex:** male
**Strain:** Wistar
**Route of administration:** gavage
**Exposure Period:** 14 days
**Frequency of treatment:** daily
**Duration of test:** 14 days
**Doses:** 1 mmol/kg/day
**Control Group:** yes, concurrent vehicle

**Method:** other: see text
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Following repeated oral administration of equimolar dose levels of various alkanols to male rats for a period of 14 days there were no statistically significant differences in body weight gain, or relative liver or testes weights.
**Source:** Rhodes, 1984
Hayes Consultancy Service Bromley, Kent
**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce similar effects to those observed with diethyl hexyl phthalate (DEHP) and its metabolite 2-ethyl hexanol in terms of hepatomegaly, peroxisome proliferation, hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any

indication of testicular atrophy (a known effect of DEHP).

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol as a vehicle at a common dose level (on a molar basis) of 1 mmol/kg/day for 14 days. At the end of this period testes weights were recorded together with various indices of liver toxicity (see chapter 5.4 Repeated dose toxicity for further details).

Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day

**Test substance:** Tradename Synprol C13-15 C10-16 alcohols Type D

Various alkanols were tested as follows:

Branched alcohols
2-ethyl hexanol C8
Iso-octanol C8
3,5,7-trimethylhexanol C9
Iso-nonanol C9
Iso-decanol C10
Tridecanol C13

Mixed branched & straight chain
Alphanol C7-9
Synprol C13-15 CAS RN 67762-41-8

Straight chain
Alfol C6-10 (Alfol 610) C6-10 (even) CAS RN 64365-05-5
Linevol C7-9 (Linevol 79) (odd) CAS RN 68603-15-6 (85% linear)
85% linear.

**Conclusion:** The results of this study provide supportive evidence for a lack of effect of a range of alcohols on the testes following repeated oral administration as evidenced by lack of effect on relative testes weights.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

20-JUL-2005 (35)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C10-16 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for developmental toxicity is based are either comparable to guideline or similar studies or publications with sufficient detail for assessment.

18-OCT-2005 (51) (52) (56)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

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(6) Biolab SGS 1991f Acute eye irritation Alchem 123. Protocol NO. 5683/3 dated 28.10.91

(7) Biolab SGS 1991g Acute eye irritation Isalchem 123 Protocol 5683/1 dated 28.01.91

(8) Biolab SGS, 1991b Primary irritation Lial 123. Protocol No. 5683/3 Summary report, 1991

(9) Biolab SGS, 1991c Primary irritation Alchem 123. Protocol No. 5683/3 Summary report, 1991

(10) Biolab SGS. 1990a. Acute oral toxicity ALCHEM 123.

(11) Biolab SGS. 1991a. Primary skin irritation Isalchem 123, Protocol 5683/1. Summary report dated 28.01.91.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 68551-07-5
**CAS No.** 68551-07-5
**EINECS Name** Alcohols, C8-18
**EC No.** 271-359-0

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
**Revision date:**
**Date of last Update:** **08-MAR-2006**

**Number of Pages:** **36**

**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

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**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491 828557

08-MAR-2006

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** West Lathrop Avenue P.O. Box 2668
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Konrad Gamon **Date:**
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**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium member
08-MAR-2006

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome Minato-ku
**Town:** 100-0005 Tokyo
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**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** 1-8, 2-Chome, Bingo-Machi
**Town:** 541-0051 Osaka
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**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
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**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium member
08-MAR-2006

**Type:** cooperating company
**Name:** Sasol Italy S.p.A.
**Contact Person:** Enrico Dallara **Date:**
**Street:** V. Medici del Vascello, 26
**Town:** 20057 20138 Milano
**Country:** Italy

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. Dave Penney **Date:**
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**Country:** United States

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** SASOL Olefins and Surfactants GmbH
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**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** The Procter and Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
08-MAR-2006

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
04-AUG-2005

## 1.0.3 Identity of Recipients

**-**

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| Chemical name | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |

Alcohols, C12-14 80206-82-2
Alcohols, C8-10 85566-12-7
Alcohols, C10-12 85665-26-5
Tridecanol, branched and linear 90583-91-8
Alcohols, C18-22 97552-91-5

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C8-18 alcohols, CAS 68551-07-5 are 100% linear.

The substance comprises 5-30% C8 and 10, >60% C12, 14, 16 and 18. Components of even chain length, in the range C8-C20 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C8-18
Alkanols, C8-18
C8-18 alcohols
C8-18-fatty alcohols
Fatty (C8-C18)alcohol
Oxo alcohol still bottoms

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C8-18 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >250 - 500 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >500 000 - 1 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (5) (8) (13)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

-

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG or 1 ID No. 1482 and 656
05-AUG-2005 (15)

### 1.8.4 Major Accident Hazards

-

### 1.8.5 Air Pollution

-

### 1.8.6 Listings e.g. Chemical Inventories

-

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-16 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

-

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
23-AUG-2005 (1)

## 2.2 Boiling Point

**Value:**

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
**Reliability:** (2) valid with restrictions
23-AUG-2005 (1)

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (12)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000019 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
19-SEP-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 3.2 - 7.2 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.
Dissociation is not expected under normal conditions of pH (pKa expected to be >15). A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 26.5 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the

SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 26.5 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
13-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** = 128 degree C
**Type:** open cup

**Method:** other: Cleveland method
**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
This information was obtained from secondary literature (company MSDS)
11-OCT-2005 (9)

## 2.8 Auto Flammability

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## 2.9 Flammability

-

## 2.10 Explosive Properties

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## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

### 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
13-SEP-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4.

However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint
13-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation)
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**
TGD Hydrophobics method: Koc = 448 - 839000
TGD Non-hydrophobics method: Koc = 460 - 57400
TGD Alcohols method: Koc = 54 - 2010
SRC PCKOCWIN method: Koc = 28 - 12900

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, though the ten-day window may not be met. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS

dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

**Type:** aerobic
**Inoculum:** other bacteria: Pseudomonas sp. (adapted)
**Concentration:** 800 µmol/l related to Test substance
**Degradation:** ca. 70 % after 2 day(s)

**Remark:** Alkohole (C10 - C18) als Gemisch geprueft; Einzel-Abbauraten aus GC-Peaks bestimmt; Abbau-Werte aus Graphik ermittelt
**Source:** Henkel KGaA Duesseldorf
**Test condition:** Inkubation in Minimalmedium mit Gemisch aus Alkoholen (C10, C12, C14, C16 & C18) in Konzentrationen zu je 0.8 mmol/l; geschuettelt; T = 30 Grad C
**Reliability:** (3) invalid
This information was obtained from the public IUCLID 2000 CD-ROM. A source of higher reliability is available. Adaptation of the inoculum is a significant methodological deficiency and it is very likely that this result would be invalid. Further review of the original source, to confirm the reliability, would not alter the overall conclusions concerning this end point.
05-OCT-2005 (16)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 95 - 43800

**Method:** other: other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions

The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 3.6

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 1.3

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

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## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

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### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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### 4.7 Biological Effects Monitoring

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### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty

acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (6)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22) including data for C8 (1-octanol), C10 (1-decanol), C12 (1-dodecanol), C14 (1-tetradecanol), C16 (1-hexadecanol), and C18 (1-octadecanol) alcohols, which support the statement that C8-18 alcohols are expected to be of low acute oral toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (10) (11) (14)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C8 (1-octanol), C8-10, C10 (1-decanol), C12 (1-dodecanol), C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18 and C20 (eicosanol) alcohols in support of the statement that C8-18 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (10) (11)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20) including data for C8 (1-octanol), C10 (1-decanol), C12 (1-dodecanol), C14 (1-tetradecanol), C16 (1-hexadecanol), C16-18 and C20 (1-eicosanol) alcohols, which support the statement that C8-18 alcohols are expected to be

of low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (10) (14)

### 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. Lower members of the sub-category of linear alcohols (C6 - C11) have a skin irritation potential in the range mild - irrritant, when applied undiluted for 4 - 24 hours, while the skin irritation potential of the longer chain members (C12 and above) can be categorised as mild - essentially non-irritant. These alcohol cuts can contain up to 30% of the lower molecular weight alcohols (C8/C10) and it is therefore expected that they may be irritating to the skin. Data are available for C8 (1-octanol), C9 (1-nonanol), C10 (1-decanol) and C11 (undecanol), C12 (1-dodecanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) alcohols which support the conclusion that C8-18 alcohols are expected to be irritating to the skin.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** C8-18 alcohols are expected to be irritating to the skin.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (10) (11) (14)

### 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants of the categories 2A or 2B while alcohols of chain length >C12 are essentially non-irritating to the eye. Data are available for C8 (1-octanol), C9 (1-nonanol), C10 (1-decanol) and C11 (undecanol), C12 (1-dodecanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) alcohols. C8-18 alcohols can contain up to 30% of the lower molecular weight alcohols (C8/C10) and it is therefore expected that they may be irritating to the eye.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** C8-18 alcohols are expected to be irritating to the eye.
**Reliability:** (2) valid with restrictions

The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C6 (hexanol), C12 (dodecanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C8-18 alcohols are not expected to be skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

05-DEC-2005 (10) (11) (14)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C8-18 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro

testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-to-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C8-18 alcohols are available from studies of reliability 1 or 2 for 1-octanol, 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, tetradecanol, hexadecanol and octadecanol[Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol, dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (7) (10) (11) (14)

## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear

alcohols.

Data in support of the conclusion that C8-18 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol), C18 (octadecanol) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (7) (10) (10) (11)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C8-18 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.8.3 Toxicity to Reproduction, Other Studies

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## 5.9 Specific Investigations

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## 5.10 Exposure Experience

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## 5.11 Additional Remarks

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(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(5) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(6) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

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(8) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(9) MSDS for Kalcol A; Kao Corporation; KCDS number 100012-06, dated 26th August 2005

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(11) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

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(13) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

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(15) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

(16) Williams, J. P. et al., Appl. Microbiol. 14, 156-160 (1966)

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 68002-94-8 |
| **CAS No.** | 68002-94-8 |
| **EINECS Name** | Alcohols, C16-18 and C18-unsatd. |
| **EC No.** | 268-106-1 |
| **TSCA Name** | Alcohols, C16-18 and C18-unsatd. |

| | |
|---|---|
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
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| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

04-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Consortium Member
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
08-MAR-2006

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20057 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Susan Antrican **Date:**
**Street:** Ms. Susan O. Antrican, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C16-18 and C18 unsaturated alcohols, CAS 68002-94-8 are 100% linear.

The substance comprises >70% C16 and C18, <10% C14, including 40-90% C18 unsaturated alcohols. Components of even chain length, in the range C12-C22 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required

11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C16-18 and C18-unsatd. (CA INDEX NAME)
Alcohols, fatty, C16-18 and C18-unsatd.
Henkel 3318

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C16-18 and C18 unsaturated alcohols.

Composition is described in section 1.1.1, General Substance Information

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 - 250 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 - 500 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.
21-DEC-2005 (4) (42) (49)

## 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

## 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 658.
05-AUG-2005 (51)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C16-18 and C18 unsaturated alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

11-AUG-2003

## 2.1 Melting Point

**Remark:** solidification range: 28 - 34 degr. C
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (8)

**Remark:** Solidification range: 2 - 21 degr. C
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (44)

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
19-SEP-2005 (1)

## 2.2 Boiling Point

**Value:** = 315 - 360 degree C at 1013 hPa

**Method:** other: DIN 51751

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (44)

**Value:** = 330 - 360 degree C at 1013 hPa

**Method:** other: DIN 51751

**Remark:** Exact boiling point is dependent on composition, i.e. percentage of unsaturated alcohols.
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (44)

**Value:**

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** = .83 - .84 g/cm³ at 40 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005 (44)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No reliable measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (47)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000037 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 6.7 - 7.2 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The substance has a range of components, as described in section 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .045 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.045 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** at 20 degree C
**Descr.:** not soluble

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (44)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 170 degree C
**Type:** closed cup

**Method:** other: DIN 51758

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (44)

**Value:** ca. 190 degree C
**Type:** closed cup

**Method:** other: DIN 51758

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
17-OCT-2005 (44)

## 2.8 Auto Flammability
-

## 2.9 Flammability
-

## 2.10 Explosive Properties
-

## 2.11 Oxidizing Properties
-

## 2.12 Dissociation Constant
-

## 2.13 Viscosity
-

## 2.14 Additional Remarks
-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure).

Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint

13-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance.

The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 96500 - 839000 |
| TGD Non-hydrophobics method: | Koc = 30100 - 57400 |
| TGD Alcohols method: | Koc = 1240 - 2010 |
| SRC PCKOCWIN method: | Koc = 3790 - 12900 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods

28-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: suspension of garden soil
**Concentration:** 2 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 87 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**

| | |
|---|---|
| 5 day(s) | = 50 % |
| 15 day(s) | = 80 % |
| 28 day(s) | = 87 % |

**Method:** other: EEC Directive 79/831/EEC part C.4-E (corresponds to OECD 301D)
**Year:** 1999
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier, tetrapropylenebenzenesulfonate. The proportion of test substance to emulsifier was 1:2.5. A 5 mg/l concentration test substance was also used, however the oxygen capacity of the test bottles was not sufficient for a complete biodegradation and the results are not given.

The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.

**Result:**

The substance degraded >60% over the test period. Insufficient information is reported to confirm whether the 10 day window criterion was met but since 50% degradation was attained by day 5, the substance is considered to be readily biodegradable.
Kinetic of control substance:
5 days = 54%
15 days = 80%
28 days = 91%

**Test condition:** Inoculum concentration: not reported
Test volume: not reported
Temperature: not reported
pH: not reported

**Reliability:** (2) valid with restrictions
Study not conducted to GLP and uses a non-standard inoculum. Some experimental details are not reported.

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (7)

**Type:** aerobic
**Inoculum:** other: effluent from predominantly domestic sewage treatment plant
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 30 day(s)
**Degradation:** = 78 % after 30 day(s)
**Result:** readily biodegradable
**Kinetic:** 15 day(s) = 17 %
30 day(s) = 78 %
**Control Subst.:** other: not reported.

**Method:** other: RDA-Blok-Test
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test method used is based on the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken. The method is suitable for poorly water-soluble compounds and corresponds to the ISO/DIS method 10708.

**Remark:** The summary report states test chemical concentration was 100 mg COD/l in the test procedure but 50 mg COD/l in the results section.
This information is from a 1 page summary of the full report. No information is provided regarding the validity criteria.
**Result:** Degradation values reported for days 15 and 30 only. Test chemical degraded by 70% after 15 days. The test chemical appears readily biodegradable, although insufficient information is reported to confirm if the 10-day window criterion was met.
**Reliability:** (4) not assignable
Summary report only available for review. No information reported on reference material or validity criteria for the test.
28-SEP-2005 (34)

**Type:** anaerobic
**Inoculum:** anaerobic sludge
**Concentration:** 50 mg/l related to Test substance
**Contact time:** 84 day(s)
**Degradation:** = 89 % after 84 day(s)
**Result:** other: easily biodegradable under anaerobic conditions

**Method:** ECETOC Anaerobic biodegradation
**Year:** 1992
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Anaerobic biodegradability testing was carried out in the ECETOC Anaerobic Biodegradation Test (Birch et al.,1989). A known volume of anaerobic sludge obtained from a municipal wastewater digester is suspended in an oxygen-free medium in a vessel where gases can evolve in the headspace. The test material is added. There are five replicates for the test material and the control. The vessels are incubated at 35 degrees C for up to 8 weeks. The headspace pressure is measured once a week and the dissolved inorganic carbon (DIC) content of the digester liquor is determined at the end of the test. The extent of anaerobic ultimate degradation is calculated by comparison of the amount of carbon equivalent to net gas and DIC production with the initially added organic carbon content of the test chemical. ECETOC Screening Test (Technical Report 28, June 1988) which is equivalent to ISO International Standard 11734. Water quality - Evaluation of the "ultimate" anaerobic biodegradability of organic compounds in digested sludge - method by measurement of the biogas production. International Organization of Standardization. 1994.
**Result:** Digester gas formation ($CH_4$) in % of applied organic carbon (corrected for control):
7 days = 25.1%
28 days = 47.8%
49 days = 55.7%
70 days = 60.1%
84 days = 61.1%
Dissolved inorganic carbon ($CO_2$) in % of applied organic carbon at end of test (corrected for control): 27.5%
Total anaerobic degradation: 88.6%

**Test condition:** Inoculum concentration: >1 - <4 g of dry suspended solids (DSS) per litre
Test volume: 500 ml
Temperature: 33-37 C
pH: 6.8-7.1
**Reliability:** (1) valid without restriction
Best study although not a SIDS endpoint.
07-JAN-2005 (32) (48)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 2 mg/l
**Degradation:** >= 30 % after 30 day(s)

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** EG-RiLi 84/449 Anh.V C4-E
**Remark:** Lösungsvermittler eingesetzt
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 2 mg/l referring to Active Substance: 40% with parameter % BSB/CSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (21) (25)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 2 mg/l
**Degradation:** = 100 - 80 % after 30 day(s)

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** EG-RiLi 84/449 Anh.V C4-E
**Remark:** Lösungsvermittler eingesetzt 2 ppm: Abbau > 100% ungenügender Restsauerstoff in der höheren Prüfkonzentration.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 2 mg/l referring to Active Substance: 100% with parameter % BSB/CSB
#2: 5 mg/l referring to Active Substance: 80% with parameter % BSB/CSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (19) (22) (27)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 2 mg/l
**Degradation:** = 100 % after 30 day(s)

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** EG-RiLi 84/449 Anh.V C4-E
**Remark:** Lösungsvermittler eingesetzt Abbauergebnisse > 100% / Bewertung unter Vorbehalt ungenügender Restsauerstoff in der höheren Prüfkonzentration CSB nicht reproduzierbar.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 2 mg/l referring to Active Substance: 100% with parameter % BSB/CSB
**Test substance:** Active Matter = 100 %
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (20) (23) (28)

**Type:** aerobic
**Inoculum:** other: soil suspension
**Concentration:** 2 mg/l
**Degradation:** = 87 % after 30 day(s)
**Result:** readily biodegradable

**Method:** Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** EG-RiLi 84/449 Anh.V C4-E
**Remark:** Die Prüfung erfplgte in Kombination mit TBS im Verhältnis (1:2,5). Abbauergebnis: 108% BSB30/CSB; bezogen auf abgeschätzten BSBT=3,17 ergibt das o.g. Ergebnis.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 2 mg/l referring to Active Substance: 87% with parameter % BSB/ThSB
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (19) (22) (27)

**Type:** aerobic
**Inoculum:** other bacteria: aus ueberwiegend kommunalem Abwasser
**Concentration:** 2 mg/l related to Test substance
**Degradation:** = 100 % after 28 day(s)
**Result:** readily biodegradable

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"

**Year:** 1984
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (14)

**Type:** aerobic
**Inoculum:** other: municipal sewage treatment plant effluent
**Concentration:** 2 mg/l related to Test substance
**Degradation:** = 100 % after 30 day(s)

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
07-JAN-2005 (14)

**Type:** aerobic
**Inoculum:** other: sewage treatment plant effluent/biological stage
**Concentration:** 50 mg/l
**Degradation:** = 78 - 85 % after 30 day(s)
**Result:** other: well biodegradable

**Method:** other: RDA-Test according to Blok (AWU)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** AWU-Test: 1.Wert Zwischenbelüftung 2.Wert ohne Zwischenbelüftung
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Chemical oxygen demand: 78% with parameter % BSB/CSB
#2: 50 mg/l referring to Chemical oxygen demand: 85% with parameter % BSB/CSB
**Test substance:** Active Matter = 100 %
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (18) (23) (26)

**Type:** anaerobic
**Inoculum:** anaerobic sludge
**Concentration:** 50 mg/l

**Degradation:** = 86.6 % after 84 day(s)
**Result:** other: easily biodegradable under anaerobic conditions

**Method:** ECETOC Anaerobic biodegradation
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Faulschlamm aus Kläranlage Hilden.
**Source:** Henkel KGaA Duesseldorf
**Test condition:** #1: 50 mg/l referring to Active Substance: 88.6% +-14.8% with parameter
**Test substance:** Active Matter = 100 %
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
07-JAN-2005 (24)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 43800 - 45100

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.
21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC0:** = 10000
**LC50:** > 10000
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
**Remark:** This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. The test method used corresponds to OECD Guideline 203. Mortalities were recorded at 24 hour intervals. The test was carried out prior to 1999.
The solubility of the lowest carbon chain length in the compound, C16, is about 0.01 mg/l, therefore the LC50 was not achieved at the solubility limit.
**Result:** RESULTS: EXPOSED
LC50 >10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source:** Henkel KGaA 1999o.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
13-SEP-2005

**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** = 1000
**LC50:** > 1000

**Method:** other: ISO 7346/2 (semistatic)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** LC0/EC0 entspricht der höchsten Prüfkonzentration Related to: Test substance
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
20-OCT-2005 (16)

**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**LC0:** = 200
**LC50:** < 200

**Method:** other: DIN 38412, Teil 15 (Golden orfe, acute toxicity test)
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** LC0/EC0 entspricht der höchsten Prüfkonzentration
Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
28-SEP-2005 (15)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
21-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = 5
**EC50:** = 70
**EC100:** > 160
**Limit Test:** no

**Method:** other: EU Guideline 92/69/EWG

**Year:** 1995
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.
**Result:** RESULTS: EXPOSED
EC50 = 70 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 5% of control animals died after 24 hours
Nature of adverse effects: immobilisation
**Source:** Henkel KGaA 1995.
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Own breed
Feeding: Scenedesmus subspicatus
Feeding during test: No feeding according to EU Guideline
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: 0.1003 g test substance filled up to 100 ml with deionised water; dispersion with blender and ultrasound
Vehicle, solvent: Not reported
DILUTION WATER
Source: M4 medium
Alkalinity: Not reported
Hardness: Medium
Conductance: Not reported
TEST SYSTEM
Concentrations: 5/10/20/40/80/160 mg/L
Dosing rate: Once (static test)
Exposure vessel type: Not reported
Number of replicates: 2 per test substance concentration; 4 for control
Invertebrate per replicate: 10
Test temperature: 20-21 C
Dissolved oxygen: 86-97%
pH mean: 7.7 -7.9
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Yes; 0.5 mg DOC/l and 0.4 mg DOC/l measured after 48 hours for 5 and 40 mg/l dose groups respectively
**Reliability:** (2) valid with restrictions
19-OCT-2005 (33)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are

summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

**Species:** Daphnia magna (Crustacea)
**Exposure period:** 24 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 500

**Method:** other: DIN 38412, Teil 11 (Daphnia, acute toxicity test)
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Method conforms with OECD Guide-line 202, part 1
**Remark:** LC0/EC0 entspricht der höchsten Prüfkonzentration
Related to: Test substance
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
20-OCT-2005 (15)

**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC0:** = 5
**EC50:** = 40
**EC100:** > 160

**Method:** other: DIN 38412, Teil 11 (Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse, Daphnia Kurzzeittest)
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test method conforms with OECD-Guideline 202.
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
17-OCT-2005 (13)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = 10000
**EC10:** > 10000

**Method:** other
**Year:** 1988
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the inhibitory effect of waste water on the oxygen consumption of pseudomonas putida (L 27); DIN 38412 part 27.
The oxygen consumption rate of a bacterial suspension fed with glucose as nutrient base is measured after a contact time of 30 minutes. The oxygen consumption rate of the same bacterial suspension in the presence of various concentrations of a test substance under otherwise identicl conditions is also measured. The inhibitory effect of the test substance at a particular concentration is expressed as a percentage of the mean oxygen consumption rates of the controls. An EC0 value can be determined from these measurements.
**Remark:** This information is taken from a summary of the full report completed in 1998. No additional information is contained

in the summary.
The water solubility of the lowest carbon chain length of the compound is approximately 0.01 mg/l, therefore the EC50 was not achieved at the solubility limit.
**Source:** Henkel KGaA 1988a.
**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.
17-OCT-2005 (31)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** = 700
**EC10:** = 1000

**Method:** other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Method conforms with OECD Guide-line 209
**Remark:** Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
06-AUG-2005 (17)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish
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### 4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms
-

### 4.6.2 Toxicity to Terrestrial Plants
-

### 4.6.3 Toxicity to Soil Dwelling Organisms
-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species
-

## 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.
**Source:** de Wolf and Parkerton 1999.
**Reliability:** (2) valid with restrictions
30-OCT-2003 (9)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

**Result:** The addition of the test materials to the diet of the rats produced no obvious ill effects. Neither was there any marked effect on distribution of lipid classes or the fatty acid composition of the phosphoglycerides of the liver. There was however a marked change in the composition of bothe the alkyl moieties and alk-1-enyl moieties in the phosphoglycerides of rat liver.
**Source:** Bandi et al, 1971
Hayes Consultancy Service Bromley, Kent
**Test condition:** Groups of 4-5 week old rats (4/group) were fed a basic diet and other than the control group received a daily supplement of 100 mg/kg/day by gavage of each of the following:

cis-9-octadecenyl (oleyl) alcohol; cis, cis-9, 12-octadecadienyl (linoleyl) alcohol; cis-9-octdecenyl glycerol-(1) and cis, cis-9,12-octadecadienyl glycerol-(1).

The animals were killed 10 hours after the last feeding, brain, heart, liver, kidney & testes were weighed and inspected. the lipids were extracted and purified and analysed using thin layer chromatography.

The basic diet contained 6% peanut oil as the sole lipid source.
**Test substance:** cis-9-octadecenyl (oleyl) alcohol and cis, cis-9, 12-octadecadienyl (linoleyl) alcohol
**Conclusion:** This study shows that the oral adinistration of oleyl and linoleyl alcohol enter the long chain fatty alcohol cycle and are incorporated into the alkyl and alk-1-enyl moieties of phosphoglycerides of the rat liver.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
03-NOV-2004 (5)

**Result:** The results indicate that the test material was rapidly utilised for the biosynthesis of lipids in most tissues of the rat (heart, lungs, liver, intestine, kidney, brain and plasma). Most of the radioactive label was incorporated into the acyl moieties of both phospholipids and neutral lipids. The pattern of incorporation of radioactivity into the alkyl, alk-1-enyl and acyl moieties of the lipids suggested that oxidation and esterification of the resulting fatty acid to a wide variety of lipids are the predominant reactions. Acylation is observed mostly in the liver while alkylation to alkoxylipids occurred predominately in the heart. The presence of a large proportion of the dose (52%) in the lungs 1 hour after dosing and an increase in the proportion of radioactivity in acyl moieties at 24 hours suggests preferential deposition in the lungs followed by incorporation into lipids.

Radioactivity decreased most rapidly in the liver, kidneys and intestines.
**Source:** Mukherjee et al, 1980
Hayes Consultancy Service Bromley, Kent

**Test condition:** Groups of 5-9 male rats maintained on laboratory diet were injected intravenously (into the tail vein) with cis-9-[1-14C] octadecenol. The rats were killed at intervals of 1, 24, 48 and 96 hours after dosing. Lipids were isolated from major organs.
**Test substance:** cis-9-octadecenol
**Conclusion:** The test material was rapidly utilised for the biosynthesis of lipids in most tissues of the rat (heart, lungs, liver, intestine, kidney, brain and plasma).
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
03-NOV-2004 (43)

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: 25% aqueous suspension
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1981
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 14 day observation period.

CLINICAL SIGNS: Moderate sedation and piloerection were observed within 20 minutes of dosing. These effects had reversed within 24 hours. Average body weights for the male and female treatment groups increased as expected over the observation period.

NECROPSY FINDINGS: Swelling of the gastric mucosa was observed in 9/10 treated animals. There were no other gross effects on the internal organs.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: None reported.
**Source:** Henkel KGaA 1981h
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: rat (Wistar)
- Source: Winkelmann, Hanover, Germany
- Weight at study initiation: average body weight males 1584g, females 141g.
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single

- Volume administered or concentration: 20 ml/kg as a 25% aqueous suspension.
- Post dose observation period: 14 days.

EXAMINATIONS: Mortality and clinical signs were recorded immediately after dosing then at 1, 4 and 24 hours and daily thereafter throughout the observation period. Body weights were taken before dosing and at 24 hours, 1 and 2 weeks after dosing. All rats were subject to gross necropsy at the end of the observation period.

**Test substance:** Tradename HD-Ocenol 80/85

**Conclusion:** The rat oral LD50 for HD-Ocenol 80/85 was >5000 mg/kg. Transient sedation and piloerection were observed shortly after dosing. Gross pathological examination revealed swelling of the gastric mucosa.

This study is reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (30) (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA Report no. TBD 810389 (study no. 953)

Report of acute oral LD50 determination in the rat carried out to OECD Guideline 401. Result LD50 >5000 mg/kg. No other details given.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA as follows:

Rat oral LD50 >10,000 mg/kg bw Archive no. TBD 700030, 1969
Rat oral LD50 >25,000 mg/kg bw Archive no. TBD 690020 and 690025, 1969 also TBD 710079 and 740051, 1971.

Mouse oral LD50 >10,000 mg/kg bw Archive nos. TBD 700032, 1970 and 730111, 1973.
Mouse oral LD50 >20,000 mg/kg bw Archive no. TBD 720024, 1972.

No further details of these studies are available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute

inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12 (1-dodecanol), C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18, C18 (octadecanol) and C20 (eicosanol) alcohols in support of the statement that C16-18 and C18 unsaturated alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration. Ref 2, 3, 4

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (45) (46) (50)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category from C6-20). This includes data reported for c14 (tetradecanol), C16-18 alcohols and the C20 alcohol (1-eicosanol). This data supports the statement that C16-18 and C18 unsaturated alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (46) (50)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Result:** highly irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"

**Year:** 1990
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hour
- Erythema: Individual 3, 3, 2.7 group mean 2.9
- Oedema: Individual 3, 2.7, 2

REVERSIBILITY: In 2 test animals the effects had fully reversed by 7 and 14 days. All scores for erythema and oedema were 0 at day 21 but scabbing was evident in the third animal. Erythema and oedema scores were not reported for the 7 and 14 day observation points just the fact that the skin reaction had reversed or not.

**Source:** Henkel, 1990a

**Test condition:** TEST ANIMALS: rabbit
- Strain: Kleimrusse Chbb:HM
- Sex: male
- Source: Thomae, Biberach/D
- Age: 13-14 months
- Weight at study initiation: mean weight 2790 g
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Area of exposure: 6 cm2
- Occlusion: semiocclusive
- Total volume applied: 0.5 ml
- Postexposure period: 21 days

EXAMINATIONS
- Scoring system: EU
- Examination time points: 1, 24, 48 and 72 hours, 7, 14 and 21 days.

**Test substance:** Tradename HD-Ocenol 90/95

**Conclusion:** HD Ocenol 90/95 is a skin irritant according to EU criteria (group mean 24+48+72 hour score >2 for oedema and erythema) and a Class 2 irritant according to GHS criteria (individual mean 24+48+72 hours scores for oedema and erythema >2.3 in at least 2/3 test animals.

This study is reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (37) (41)

**Species:** human
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 20
**Result:** not irritating

**Method:** other: similar protocol to OECD 404
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No irritation was observed following application to the human

skin of undiluted test substance for 4 hours (patch test).
**Source:** Henkel, 1996
**Test condition:** The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.

Study was performed under Good Clinical Practice (GCP).
**Test substance:** Tradename HD-Ocenol 90/95 V
**Conclusion:** Undiluted HD-Ocenol 90/95 did not produce any skin irritation in human vounteers following a 4 hour semi-occlusive exposure in a test based on OECD 404.

This study reported in Iuclid 2000.
**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
25-OCT-2005 (12) (41)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 5
**PDII:** 2.6
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hour mean
- Erythema: individual 2, 2.3, 1, 1.3, 0.3 Group mean 1.4
- Edema: 1.3, 1.3. 1.3, 2, 0 Group mean 1.2

REVERSIBILITY: By day 7 all scores were 0 however the skin showed desquamation in 4/5 rabbits. By day 10 the irritation had completely reversed.
**Source:** Henkel, 1987
**Test condition:** TEST ANIMALS: rabbit
- Strain: Kleimrusse Chbb:HM
- Sex: male
- Source: Thomae, Biberach/D, Germany
- Weight at study initiation: mean weight 2402 g
- Number of animals: 5

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted (warmed slightly)
- Area of exposure: 2.5 cm2
- Occlusion: occlusive
- Total volume applied: 0.5 ml
- Postexposure period: 10 days

EXAMINATIONS

- Scoring system: EU
- Examination time points: 1, 24, 48 and 72 hours, 7 and 10 days.

**Test substance:** Tradename Ocenol 50/55

**Conclusion:** Ocenol 50/55 is not a skin irritant according to EU criteria. This test substance might be considered a mild irritant category 3 according to GHS criteria as 3/5 test rabbits had mean 24+48+72 hour erythema or oedema scores of >=1.5.

This study is reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (35) (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel Archive nr. TBD 710038, 1971

In a rabbit patch test 25% aqueous HD-Eutanol was placed on one side of the dorsal surface and 50% on the other.

Result: The 25 % solution produced visbible redness at 2 test sites increasing after 24 hours. There were no initial findings at the 2 other test sites but after 24 hours there was clear redness. With the 50% solution all 4 test sites showed initial visble redness increasing to clear redness at 24 hours.

In a human patch test there was no irritation (test substance & concentration not defined).

**Test substance:** Tradename HD Eutanol

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data reported ex Henkel KGaA Archive Nr. 690025, 1969 and TBD 690020, 1969

Twice daily application of the test substance to rabbit and guinea pig skin caused irritation. No other details available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel of various studies in hairless mice (and rats) as follows:

Archive nr. TBD 700050, 1970
TS massaged twice daily into the skin. Result Irritating.

Archive nr. TBD 690020, 1969
1. Twice daily application. Result: slightly irritating -

wrinkling of skin slightly increased.
2. No experimental details. Result: irritating - marked scaling and roughness.
3. Twice daily application (rats). Result: slightly irritating - slight scaling observed.

Archive nr. TBD 700093, 1979
TS massaged twice daily into the skin. Result slightly irritating.
No further experimental details or details of the test substance available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

**Species:** human
**Concentration:** undiluted
**Exposure:** Open
**No. of Animals:** 20

**Method:** other: Burckhardt test, open epicutaneous
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No irritating effects or subjective sensations were observed.
**Source:** Henkel, 1996a
**Test condition:** The effect on human skin was investigated:
Undiluted test substance was applied to the forearm with a glass rod for a total application period of 60 minutes. Every 30 seconds, the test substance was gently swabbed with tissue and new test substance applied. Objective findings (erythema, edema) and subjective sensations (e.g. itching, cauterization etc.) were recorded after 15, 30, 45 and 60 minutes.
20 male and female volunteers of average age 35.3 years were tested.
**Test substance:** Tradename HD-Ocenol 90/95 V
**Conclusion:** HD-Ocenol 90/95 V was not irritating to human skin following repeated application to non-occluded skin over a period of 1 hour.
**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

25-OCT-2005 (39)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1990
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual 0.1, 0, 0 mean 0.03
- Conjunctivae (Chemosis): 0
- Overall irritation score: non-irritant

DESCRIPTION OF LESIONS: Slight redness (1) with some discharge in all animals at 1 hour. All eyes were normal at 24 hours.

REVERSIBILITY: Fully reversible.

**Source:** Henkel, 1990b

**Test condition:** TEST ANIMALS: rabbit
- Strain: Kleinrussen, Chbb:HM
- Sex: no data
- Source: Thomae, Biberach/D Germany
- Age: 6-7 months
- Weight at study initiation: mean 2600g
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: EU
- Observation period: 72 hours
- Tool used to assess score: slit lamp

**Test substance:** Tradename HD-Ocenol 90/95

**Conclusion:** HD-Ocenol 90/95 is not an eye irritant according to EU or GHS criteria.

This study has been reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (38) (41)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 other: g
**Exposure Time:** hour(s)
**Comment:** not rinsed
**No. of Animals:** 4
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual 0.1, 0, 0 mean 0.03
- Conjunctivae (Chemosis): 0
- Overall irritation score: non-irritant

DESCRIPTION OF LESIONS: Slight redness (1) in all animals at 1 and 6 hours with some discharge in 2/4 animals at 1 hour only. All eyes were normal at 24 hours.

REVERSIBILITY: Fully reversible.

**Test condition:** TEST ANIMALS: rabbit
- Strain: Kleinrussen, Chbb:HM
- Sex: no data
- Source: Thomae, Biberach/D Germany
- Weight at study initiation: mean 2228g
- Number of animals: 4

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Amount of substance instilled: 0.1 g
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: EU
- Observation period: 72 hours
- Tool used to assess score: slit lamp

**Test substance:** Tradename Ocenol 50/55

**Conclusion:** Ocenol 50/55 is not irritating to the rabbit eye.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (36)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Upublished data ex Henkel as follows:

Archive no. TBD 740081, 1969
Rabbit eye irritation. Result not irritating.

Archive no. TBD700050, 1970
Rabbit eye irritation (Draize test). Result slightly irritating.

Archive no. TBD690020 & 690025, 1969
Rabbit eye irritation (Draize test). Result not irritating.

No further experimental details available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction .1 % intracutaneous
**2nd:** Induction 15 % occlusive epicutaneous
**3rd:** Challenge 10 % occlusive epicutaneous
**No. of Animals:** 40
**Vehicle:** other: liquid paraffin
**Result:** not sensitizing

**Classification:** not sensitizing

**Method:** other: Magnusson & Kligman, 1969
**Year:** 1988
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: 0.1% caused a reasonable reaction following intracutaneous injection. 5 and 10% applied topically produced no irritation while 15% caused slight irritation.

RESULTS OF TEST
- Sensitization reaction:
Response with 5% challenge concentration:
24 hour 1/19 treated, 2/20 controls
48 hour 2/19 treated, 2/20 controls

Response with 10% concentration:
24 hour 2/19 treated, 4/20 controls
48 hour 2/19 treated, 6/20 controls

As more controls reacted than treated animals the reaction was ascribed to irritation and the test substance is not considered to be a skin sensitiser.

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: Pirbright white
- Sex: female
- Source: Interfauna, Tuttlingen, Germany
- Weight at study initiation: main study mean treated 312.4g controls 295.8g
- Number of animals: 20 treated
- Controls: 20

ADMINISTRATION/EXPOSURE
- Study type: Adjuvant study
- Preparation of test substance for induction: in liquid paraffin
- Induction schedule: Single intradermal injection at the various test sites, 24 hours later a closed patch with 1 ml of 15% test substance in liquid paraffin was applied to the site for 48 hours.
- Concentrations used for induction: 0.1%
- Concentration in Freuds Complete Adjuvant (FCA): 0.2%
- Challenge schedule: 14 days later using a 24 hour occlusive test (Square test chambers used).
- Concentrations used for challenge: 0.1 ml of a 5 or 10 % solution in liquid paraffin
- Rechallenge: No
- Positive control: not reported

Concentrations based on a pilot study.

**Test substance:** Tradename Ruebocenol SU
**Conclusion:** Ruebocenol RU is not a skin sensitiser when tested using the guinea pig maximisation assay.

This study is also reported in Iuclid 2000.

**Reliability:** (1) valid without restriction
Comparable to guideline study.

**Flag:** Critical study for SIDS endpoint

05-DEC-2005 (11) (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA Archive no. TBD 880661

Report of a maximisation test in guinea pigs, result negative. No further details available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** rat **Sex:** male/female
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 90 days
**Frequency of treatment:** daily, 5 days/week
**Doses:** 1 ml/kg bw (840 mg/kg/day)
**Control Group:** yes, concurrent vehicle
**NOAEL:** > 840 mg/kg bw

**Method:** other: An in-house protocol based on OECD Guide-line 407
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no mortality among the test animals and no adverse effects observed. Body weight gain appeared comparable between treated and control groups however there was no evidence that the results were analysed statistically. The haematological, as well as clinical-chemical parameters were comparable to the control group. The organ weights were within normal limits. No histopathological changes were reported. There was no detailed report of the measurements obtained from the various endpoints evaluated. There were no treatment related adverse effects on the liver sections examined histopathologically.
**Source:** Henkel KGaA 1973

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Weight at study initiation: 142-153g
- Number of animals: 10M+10F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 90 days
- Type of exposure: Oral gavage
- Post exposure period: None
- Vehicle: Olive oil
- Concentration in vehicle: Not reported
- Total volume applied: Not reported
- Doses: 1 ml/kg (840 mg/kg/day)

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs/mortality: daily
- Body weight: weekly

- Food consumption:
- Water consumption:
- Ophthalmoscopic examination: not reported
- Haematology: At the end of study Hb, RBC, WBC, differential bloood count
- Biochemistry: At end of study serum glucose, calcium, urea, ALAT & ASAT,
- Urinalysis: At end of study following a water loading of 2 ml/100g/bw. pH, specific gravity, glucose, albumin, blood, bilirubin, ketones, urinary sediments.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: An autopsy was carried out. Major organs were preserved. Organ weights were recorded (no further details of which organs were weighed).
- Microscopic: The liver was examined histologically following staining with both routine H&E and Sudan 111 to detect fatty degeneration.

STATISTICAL METHODS: Not reported

**Test substance:** Tradename HD-Eutanol

**Conclusion:** Repeated exposure for 13 weeks to 1 ml/kg/day (840 mg/kg) Eutanol HD appeared to have little adverse effect on the test animals. This dose level can be considered a NOAEL. The study is limited by lack of detailed reporting of the test results. The study is not in full accordance with OECD 407 but appears well conducted.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Based on guideline but limited reporting appears reasonably conducted. Lack of statistical analysis.

**Flag:** Critical study for SIDS endpoint

04-JAN-2006 (29) (41)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Bacterial reverse mutation assay
**System of testing:** Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538
**Concentration:** 8, 40, 200, 1,000, 5,000 ug/plate
**Cytotoxic Concentration:** 5000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1989
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: There was no increase in reverse mutation rate in any of the tester strains at any dose level. Positive and negative controls showed an appropriate response.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:

- With and without metabolic activation: 5000 ug/plate evidenced by reduced background lawn and/or reduced revertant rates.

**Test condition:** METHOD: OECD 471 Only 2-aminoanthracene was used as a positve control in the presence of S9.

TEST SYSTEM:
- Species/cell type: Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 8, 40, 200, 1,000, 5,000 ug/plate
- Number of replicates: Two independent tests each conducted in triplicate.
- Application: Plate incorporation assay, vehicle aqueous suspension with Tween 80.
- Positive and negative control groups and treatment: With S-9 2-aminoanthracene (2.5 or 5 ug/plate); Without S-9 9-aminoacridine (80 ug/plate), sodium azide (2ug/plate), 4-nitro-o-phenylene diamine (40 ug/plate)
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A two fold increase in reverse mutation rate is considered positive in strain TA 100 and a 3 fold increase positive for the other strains.

**Test substance:** Tradename HD-Ocenol 90/95

**Conclusion:** HD-Ocenol 90/95 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 5000 ug/plate. Evidence of cytotoxicity was observed at 5000 ug/plate (highest dose level tested).

This study is reported in Iuclid 2000

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

06-AUG-2005 (6) (41)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA Archive no. TBD 820117 pb Wa 298 and Archive no. TBD 820121 Pb Wa 302

Two Ames tests reported

Test organisms Salmonella typhimurium strains with and without metabolic activation. Concentration 4, 20, 100, 500 and 2500 ug/plate. Result: negative

No other details available.

**Reliability:** (4) not assignable
Secondary report of unpublished data.

06-AUG-2005 (41)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (40) (45) (46) (50)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C16-18 and C18 unsaturated alcohols are not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol), C22 (docosanol) and the supporting substance C18 (octadecanol).

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (45) (46) (50)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C16-18 and C18 unsaturated alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (45) (46) (50)

### 5.8.3 Toxicity to Reproduction, Other Studies

-

### 5.9 Specific Investigations

-

### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

**Remark:** The purpose of this study was to introduce the chamber-scarification test designed for increased sensitivity for assessing the irritancy of materials. It is important to note that persons especially vulnerable to irritants were selected.

The materials were applied as a 25% solution in mineral oil. The skin is first scarified and the test material applied (0.1 ml) in a test chamber once daily for 3 days to groups of 5-10 volunteers. The skin was assessed 30 minutes after the end of the final exposure.

The degree of irritation was related to carbon chain length, the C10 and C12 alcohols giving a marked response while the C14 alcohol gave a moderate response, C16 slight and the oleyl alcohol gave a low response.

**Source:** Frosch & Kligman, 1976
Hayes Consultancy Service Bromley, Kent
**Test substance:** oleyl alchol, hexadecyl alcohol, tetradecyl alcohol, dodecyl alcohol, decyl alcohol
**Reliability:** (2) valid with restrictions

06-AUG-2005 (10)

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) Bandi, Z.L. et al, 1971 The alkyl and alk-1-enyl glycerols in the liver of rats fed long chain alcohols or alkyl glycerols. FEBS Letters 12(4):217-220

(6) Banduhn, N. 1989. HD-Ocenol 90/95. Pruefung auf Mutagenitaet im Ames-Test. Institut fuer Toxikologie, Henkel KGaA. Report No. TBD 890398.

(7) Borner. 1999. HD Ocenol 80/85: Ultimate biodegradability in the closed bottle test. Biological Research/Product Safety Department of Ecology, Henkel KGaA Report No. R 9900110.

(8) data sheet, Henkel KgaA

(9) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(10) Frosch, P.J. and Kligman, A.M. 1976. The chamber-scarification test for irritancy. Contact Dermatitis 2:314-324.

(11) Henkel 1988f Ruebocenol SU Pruefung auf sensibilisierende Eigenshaften. Br. nr. 880804

(12) Henkel KGaA, 1996 HD-Ocenol 90/95 V, Lorol C12-98, Lorol-C14-98, Lorol Spezial. 4h Patch Test (in Anlehnung an OECD Guideline Nr. 404). Henkel KGaA 1996, Report No. R 9601427

(13) Henkel KGaA, unpublished data (Pruefnr. 9300287-23)

(14) Henkel KGaA, unpublished data (Registry No. 6802)

(15) Henkel KGaA, unpublished data, File 400/2

(16) Henkel KGaA, unpublished data, File 404/1, and Henkel KGaA, unpublished data, Final Report 832144

(17) Henkel KGaA, unpublished data, File 427/1;

Henkel KGaA, unpublished data, Final Report 832144

(18) Henkel KGaA, unpublished data, File 5, Page/Assay 37

(19) Henkel KGaA, unpublished data, File 57, Page/Assay 661

(20) Henkel KGaA, unpublished data, File 63, Page/Assay 775

(21) Henkel KGaA, unpublished data, Final report

(22) Henkel KGaA, unpublished data, Final report 1983 2128

(23) Henkel KGaA, unpublished data, Final report 1986 2491

(24) Henkel KGaA, unpublished data, Final report RE 920168

(25) Henkel KGaA, unpublished data, Protocol 2, Page/Assay 18

(26) Henkel KGaA, unpublished data, Protocol 2, Page/Assay 37

(27) Henkel KGaA, unpublished data, Protocol 31, Page/Assay 661

(28) Henkel KGaA, unpublished data, Protocol 33, Page/Assay 775

(29) Henkel KGaA. 1973. C16-18 alcohols, C18 unsaturated: Evaluation of repeated dose oral toxicity. Unpublished data, Report No. TBD 730054. HD-Eutanol. English summary, 1999. R9901617

(30) Henkel KGaA. 1981h. C16-18 alcohols, C18 unsaturated: Evaluation of acute oral toxicity. Unpublished data, report no. TBD 810369 (pub. no. 938) and summary dated 1999.

(31) Henkel KGaA. 1988a. Biological Research and Product Safety/Ecology. Test substance registration No. 6802. Bacterial toxicity.

(32) Henkel KGaA. 1992e. Biological Research & Product Safety Ecology Department, Oleylalkohol - Anaerobe Abbaubarkeit im ECETOC-Test. Report No. RE 920168.

(33) Henkel KGaA. 1995. Alcohols, C16-18 alcohols and C18 unsaturated (HD-Ocenol 92/96): Acute daphnia toxicity. Report No. 9400262. May 1995.

(34) Henkel KGaA. 1999p. C16-18 Alcohols, C18 unsaturated: Aerobic biodegradation: RDA-test according to Blok (AWU). Biological Research and Product Safety/Ecology: Unpublished results; test substance registration No. Fi 6802, test run No. 37.

(35) Henkel, 1987a KGaA Ocenol 50/55 (Oleyl-Cetylalkohol C16/18) Pruefung auf primaire Hautirritation. Archive nr TBD 870520 Br nr 870521.

(36) Henkel, 1987b Ocenol 50/55 (Oleyl-Cetylalkohol C16/18) Pruefung auf primairen Schleimhautirritation am Kaninchenauge. Br nr 870641.

(37) Henkel, 1990a HD Ocenol 90/95 Pruefung auf akute Hautirritation. Archive. No. TBD900201

(38) Henkel, 1990b HD-Ocenol 90/95 Pruefung auf akute Augenirritation. Arch. NR. TBD900214

(39) Henkel, 1996a Offener Epikutan-Test nach Burckhardt HD Ocenol 90/95, Lorol C12-98, Lorol C14-98, Lorol spezial. R9601185, August 1996

(40) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(41) Iuclid 2000 European Commission - European Chemicals Bureau C16-18 and C18 unsaturated alcohols CAS RN 68002-94-8

(42) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(43) Mukherjee, K.D. et al, 1980 competing pathways in the formation of alkyl, alk-1-enyl and acyl moieties in the lipids of mammalian tissues. Eur. J. Biochem. 107:289-294, 1980

(44) Safety data sheet, Henkel KgaA

(45) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(46) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(47) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(48) Steber, J., Herold, C.P. and limia, J.M. 1995. Comparative evaluation of anaerobic biodegradability of hydrocarbons and fatty derivatives currently used as drilling fluids. Chemosphere 31:4, 3105-3118.

(49) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(50) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(51) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 68155-00-0 |
| **CAS No.** | 68155-00-0 |
| **EINECS Name** | Alcohols, C14-18 and C16-18-unsatd. |
| **EC No.** | 268-930-1 |
| **TSCA Name** | Alcohols, C14-18 and C16-18-unsatd. |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **18-JAN-2006** |
| **Number of Pages:** | **36** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

23-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Consortium Member
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
19-SEP-2005

## 1.0.3 Identity of Recipients

**-**

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.
The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |

| | |
|---|---|
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential.
Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C14-18 and C16-18-unsaturated alcohols, CAS 68155-00-0 are presumed to be linear though this is not specified.
The substance comprises 5-50% C16 and 18 saturated, 40-90% C16 and 18 unsaturated. Components of even chain length, in the range C14-C18 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C14-18 and C16-18-unsatd. (CA INDEX NAME)
**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C14-18 and C16-18 unsaturated alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (4) (6) (10)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final

products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

-

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 658.

05-AUG-2005 (12)

## 1.8.4 Major Accident Hazards

-

## 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

-

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C14-18 and C16-18 unsaturated alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7

04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.

19-SEP-2005 (1)

## 2.2 Boiling Point

**Value:**

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.

19-SEP-2005 (1)

## 2.3 Density

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint

21-OCT-2005 (9)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .000019 hPa at 25 degree C

**Method:** other (calculated): from composition

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
19-SEP-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 6 - 7.2 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2005
**GLP:** no

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.
Dissociation is not expected under normal conditions of pH (pKa expected to be >15). A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
21-JUL-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** .024 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** Result: The water solubility is estimated to be 0.024 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
19-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4.However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant

substances (see section 1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
13-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** TGD Hydrophobics method: Koc = 96500 - 839000
TGD Non-hydrophobics method: Koc = 14300 - 57400
TGD Alcohols method: Koc = 711 - 2010
SRC PCKOCWIN method: Koc = 1110 - 12900

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
28-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. This substance is predicted to be readily biodegradable, though the ten-day window may not be met. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 33900 - 43800

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

21-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other: calculated (partition model)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (2)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

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### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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### 4.7 Biological Effects Monitoring

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### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty

acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (5)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22). This includes data reported for C16 (hexadecanol), C18 (dodecanol), C16-18 alcohols and C16-18 and C18 unsaturated alcohols. This data supports the statement that C14-18 and C16-18 unsaturated alcohols are expected to be of low acute oral toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (8) (11)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12-16, C14 (tetradecanol), C16 (hexadecanol), C16-18, and C18 (octadecanol) alcohols in support of the statement that C14-18 and C16-18 unsaturated alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (8) (11)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category from C6-20). This includes data reported for C14 (tetradecanol), C16 (hexadecanol, C18 (octadecanol), C16-18 alcohols and the C20 alcohol (1-eicosanol). This data supports the statement that C14-18 and C16-18 unsaturated alcohols are

expected to be of low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (8) (11)

### 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Remark:** Studies of DQ 1 or 2 are available for the unsaturated alcohols C18 unsaturated and C16-18 and C18 unsaturated which suggest that these alcohols have mild - irritant skin irritation potential. This supports the conclusion that C14-18 and C16-18 unsaturated alcohols are expected to be mildly irritating to the skin.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** C14-18 and C16-18 unsaturated alcohols are expected to be mildly irritant to the skin.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
25-OCT-2005 (11)

### 5.2.2 Eye Irritation

**Remark:** Studies of DQ 1 or 2 are available for the unsaturated alcohols, C18 unsaturated and C16-18 and C18 unsaturated, which suggest that these alcohols are non irritating to the skin. Data for C16 (hexadecanol) and C18 (octadecanol) also indicated lack of eye irritancy potential. This supports the conclusions that C14-18 and C16-18 unsaturated alcohols are expected to be essentially non-irritating to the eye.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** C14-18 and C16-18 unsaturated alcohols are expected to be essentially non-irritating to the eye.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (8) (11)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of

this category from C6-C18. Included are negative data from guinea pig maximisation tests for, C14 (tetradecanol), C16 (hexadecanol), C18 (octadecanol) and C16-18 and C18 unsaturated alcohols which support the conclusion that C14-18 and C16-18 unsaturated alcohols are not expected to be a skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

05-DEC-2005 (8) (11)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C18 unsaturated alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol), C16-18 and C18 unsaturated alchols, C18 (octadecanol) and C20 (docosanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (8) (8) (11)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C14-18 and C16-18 unsaturated alcohols are available from studies of reliability 1 or 2 for C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, C16-18 and C18 unsaturated, hexadecanol and octadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (7) (8) (11)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, C16-18 and C18 unsaturated, hexadecanol and octadecanol [Ames].

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
15-SEP-2005 (7) (8) (11)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C14-18 and C16-18 unsaturated alcohols are not expected to impair fertility are provided, in addition to the negative reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types

B&D), C14-16 (type A), C16 (hexadecanol), C22 (docosanol) and the supporting substance C18 (octadecanol).
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (7) (8) (11)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C14-18 and C16-18 unsaturated alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
15-SEP-2005 (7) (8) (11)

### 5.8.3 Toxicity to Reproduction, Other Studies

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### 5.9 Specific Investigations

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### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(6) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(7) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(8) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(9) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(10) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(11) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(12) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 68333-80-2
**CAS No.** 68333-80-2
**EINECS Name** Alcohols, C14-16
**EC No.** 269-790-4

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

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20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C14-16 alcohols, CAS 68333-80-2 are 5-95% linear.

The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C11-C16 are present.

Commercial products marketed under this CAS number fall into two types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A and Type B.

Type A products are 5-95% linear. The substance comprises >95% C14 and 15. Components of even and odd chain length, in the range C12-C17 are present.

Type B products are <=5% linear. The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C11-C16 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C14-16 (CA INDEX NAME)
C14-16 alcs.
Isalchem 145

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C14-16 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in

range C12-18)- This is publicly-available CEH data for Japan, for 2002.
21-DEC-2005 (4) (26) (31)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG ID No. 656.
05-AUG-2005 (33)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C14-16 alcohols. There could also be exposure from private use (for consumer products).
Not required
05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760
11-AUG-2003

## 2.1 Melting Point

**Value:** = 29 - 32 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**Method:** other: ASTM D97
**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** = 280 - 295 degree C at 1013 hPa
**Decomposition:** no

**Method:** other: ASTM D1078
**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** = .815 - .825 g/cm³ at 40 degree C

**Method:** other: ASTM D1298
**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No reliable measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
21-OCT-2005 (30)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00011 - .00051 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.00011 hPa
Type B: 0.00051 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** ca. 1 hPa at 125 degree C

**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 5.4 - 6.4 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of Ph (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Result:** Type A: 6.0 - 6.4
Type B: 5.4 - 6.4
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured or estimated values for the components.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (1)

**Partition Coeff.:** octanol-water
**log Pow:** = 6

**Source:** Shell Chemicals UK Ltd Chester [unreferenced]
**Test substance:** It is not possible to establish the compositional Type of the test substance.
**Reliability:** (4) not assignable

This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .7 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (15)

**Solubility in:** Water
**Value:** = .15 - .64 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.15 mg/l at a loading rate of 1000 mg/l
Type B: 0.64 mg/l at a loading rate of 1000 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** < .01 vol%

**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 152 degree C
**Type:** closed cup

**Method:** other: ASTM D93
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

### 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

### 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section

1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
13-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** Type A:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 96500 - 177000 |
| TGD Non-hydrophobics method: | Koc = 14300 - 23100 |
| TGD Alcohols method: | Koc = 710- 1020 |
| SRC PCKOCWIN method: | Koc = 1110 - 2050 |

Type B:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 177000 |
| TGD Non-hydrophobics method: | Koc = 6420 - 23100 |
| TGD Alcohols method: | Koc = 390 - 1020 |
| SRC PCKOCWIN method: | Koc = 330 - 2050 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 45.4 mg/l related to Test substance
**Contact time:** 49 day(s)
**Degradation:** = 82 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**

| | |
|---|---|
| 6 day(s) | = 12 % |
| 19 day(s) | = 70 % |
| 28 day(s) | = 82 % |

49 day(s) = 90 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: OECD Guide-line 301 F and ISO 9408
**Year:** 1995
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were met: (1) oxygen uptake of inoculum blank at day 28 was 14.5 (less than 60 mg/l), (2) the difference between replicate values of test chemical at day 28 was 9.7% (less than 20%), and (3) percentage degradation of reference compound reached 60% on day 4 (before day 14).

**Result:**
The substance had degraded >60% at the end of the test period and the 10-day window criterion was met. The lag phase was 5 days.
Kinetic of control substance: 6 days = 69%
19 days = 92%
28 days = 93%
49 days = 99%

**Test condition:** Inoculum concentration: 30 mg/l suspended solids
Test volume: 500 ml
Temperature: 18-25 C
pH: not reported

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
13-SEP-2005 (22)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 45 mg/l related to Test substance
52 mg/l related to Test substance
**Contact time:** 44 day(s)
**Degradation:** = 75 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 12 day(s) = 10 %
19 day(s) = 58 %
26 day(s) = 71 %
30 day(s) = 80 %
44 day(s) = 85 %
**Control Subst.:** other: Sodium benzoate

**Method:** other: OECD 301F and ISO 9408
**Year:** 1993
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Report states that 75% degradation had occured after 28 days of incubation. Reported degradation values were only presented for days 26 and 30.

The following validity criteria were met (1) Parallel assays did not differ by more than 20%, (2) the reference substance reached the pass level within 14 days, (3) O2 uptake in the inoculum blank was less than 60 mg O2/l after 28 days.

**Result:** Kinetic of control substance:
5 days = 81%
19 days = 91%
26 days = 90%
30 days = 93%
44 days = 89%
The test substance attained 71% degradation in 26 days but did not meet the 10 day window criterion, therefore it cannot be considered readily biodegradable.
**Test condition:** Inoculum concentration: not reported
Temperature: not reported
pH: not reported
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and higher degradation rates are available.
Guideline study conducted to GLP, but some experimental details not reported.
11-OCT-2005 (21)

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to all compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other
**Year:** 1974
**GLP:** no data
**Year:**
**Method:** The tests were conducted in accordance with the 'Standard Dilution Method' at 20 C for a period of 5 days. This method is described in APHA 'Standard Methods' Nr.219 and was formerly included in the ASTM Standards under Nr. D2329-68.

For practical reasons the official Netherlands method NEN 3255 5.4 was used. The only difference in the NEN procedure compared with the others is that consumption of oxygen as a result of nitrification is prevented by the addition of allylthiourea. The test solutions were seeded with 10 ml/l of the effluent of a biological sanitary waste treatment plant.

**Remark:** BOD measurements were expressed as weight of oxygen per weight of chemical (g/g) and, if composition of the product was known, as a percentage of the theoretical oxygen demand, ThOD (%).

**Result:** BOD 5 = 0.67 - 1.84 g/g
%ThOD = 59%
>50% degradation, therefore was grouped into good degradability class

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (2) valid with restrictions

17-OCT-2005 (16)

**Method:**

**C O D**

**Method:** other
**Year:** 1974
**GLP:** no data

**COD:** = 2.66 mg/g substance

**Method:** In the COD test (ASTM D 1252-67) the oxidizable material present in waste water is oxidised by a standard potassium dichromate solution in 50% sulfuric acid. The mixture is refluxed at about 145 C for two hours. The excess dichromate is then titrated and the COD calculated.

**Result:** The COD was found to be 2.66 g/g.
85% oxidation to water and carbon dioxide was also calculated.

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (2) valid with restrictions

17-OCT-2005 (17)

**Method:**
**Year:**

**Method:**

**Remark:** ThOD= 3.13 g O2/g substance.

**Source:** Shell Chemicals UK Ltd Chester

**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

18-JAN-2006 (25)

## 3.7 Bioaccumulation

**BCF:** = 4500 - 42600

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Result:** Type A: BCF estimated as 33900 - 42600
Type B: BCF estimated as 4500 - 42600.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods

29-DEC-2005 (3)

## 3.8 Additional Remarks

**-**

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 500
**Limit Test:** no

**Method:** other
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Five fingerlings were placed in each aquarium and mortality was recorded daily for 96 hours. The aquariums were aerated and maintained at 16 C and pH 8.0-8.4. Test concentrations were 0 (control), 3, 10, 30, 100 and 500 mg/l.
Acetone concentration was also adjusted to 1200 mg/l in each aquaria including the control.
**Remark:** The fingerlings used in this experiment weighed between 1.4 and 2.0 g. The water used in the aquaria was dechlorinated tap water.
The solubility of C14, the lowest carbon chain length in the test substance, is about 0.15 mg/l, therefore, the LC50 was not achieved at the solubility limit.
**Result:** No compound related mortality occurred when fish were exposed for 96-hours.
**Source:** Shell Toxicology Laboratory 1978b.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility are available
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (27)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 2.6 - 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown,

which follows the description given in section 1.1-1.4.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: >100 mg/l (i.e. predicted to be non-toxic at the limit of solubility)
Type B: 2.6 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
30-DEC-2005 (2)

**Type:** static
**Species:** Carassius auratus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** > .7
**Limit Test:** no

**Method:** other: ASTM Method D 1345. Test for Evaluating Acute Toxicity of Industrial Waste Water to Fresh-Water Fishes.
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test material found to be nontoxic at the saturated aqueous solution of 0.7 mg/l. The solubility of C14, the lowest carbon chain length in the compound, is about 0.15 mg/l, therefore, the LC50 was not achieved at the solubility limit.
**Result:** RESULTS: EXPOSED
LC50 >0.7 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source:** Bridie et al. 1973.
**Test condition:** TEST ORGANISMS
Strain: Carassius auratus
Supplier: Oprel, Hoogvliet, The Netherlands
Weight: 3.3 g
Feeding: Not reported
Pretreatment: Not reported
Feeding during test: Not reported
Control group: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Tap water
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Not reported
Renewal of test solution: None
Exposure vessel type: Aquaria 42x28x28 cm

Number of replicates: Not reported
Fish per replicate: 10
Test temperature: 20 C
Dissolved oxygen: 9-10 mg/l
pH mean: 6-8
Adjustment of pH: Corrected to 7.0 with NaOH or H2SO4
TEST PARAMETER: Mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (2) valid with restrictions
Other study with the same substance provides even clearer evidence of an absence of effect at a concentration that is likely to have been close to the solubility limit.

21-DEC-2005 (15)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**EC50:** = .13 - .21

**Method:** other: calculated (partition model)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.13 mg/l
Type B: 0.21 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: growth rate and biomass

**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = 4.6
**EbL50 :** = 22 - 46
**ErL50 :** = 22 - 46
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
NOEL = 4.6 mg/l
EbL50 = 22 - 46 mg/l (Area under growth curve)
ErC50 = 22 - 46 mg/l (Growth rate)
Based on loading rates
**Source:** Whale et al. 2000.
**Test condition:** TEST ORGANISMS
Strain: Raphidocelis subcapitata
Supplier: Institute of Freshwater Ecology, Windemere
Pretreatment: Not reported
Controls: 1 control group (6 replicates and 1 blank flask)
Test medium: Water Accommodated Fractions
Vehicle, solvent: None
Concentration of vehicle, solvent: None
STABILITY OF TEST CHEMICAL SOLUTIONS
Considered stable
DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0.46, 1.0, 2.2, 4.6, 10, 22, 46 and 100 mg/l
Exposure vessel type: 287 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 5000 cells/ml
Test temperature: 22.3 - 23.4
Dissolved oxygen: Not reported
pH mean: 8.7 - 10.0
Adjustment of pH: None
Intensity of irradiation: 5240 lux
Photoperiod: Under constant illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION:
At the start and end of the test period. Neodol 45E test media concentrations decreased by 67-99% over the 72 hour test period.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (34)

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For compositional Type B, for which a prediction of algal toxicity is required, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The values obtained by prediction are:
Type B: 0.1 - 1.0 mg/l

For Type A, a reliable measurement is available and therefore no estimate has been made.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (20)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

-

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in

the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (19)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | Wistar |
| **Sex:** | male/female |
| **No. of Animals:** | 5 |
| **Vehicle:** | other: undiluted |
| **Doses:** | 5000 mg/kg |
| **Value:** | > 5000 mg/kg bw |
| **Method:** | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year:** | 1990 |
| **GLP:** | no data |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: No animals died.<br><br>CLINICAL SIGNS: No signs of intoxication, no adverse effect on weight gain.<br><br>NECROPSY FINDINGS: Unremarkable.<br><br>POTENTIAL TARGET ORGANS: None identified.<br>SEX-SPECIFIC DIFFERENCES: None. |
| **Source:** | Biolab SGS 1990b<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Rat (Wistar)<br>- Source: Nossan, Correzzana, Milan, Italy<br>- Weight at study initiation: 200 g (+- 20g)<br>- Group size: 5M+5F fasted.<br>- Controls: Yes<br><br>ADMINISTRATION: gavage<br>- Doses: 5000 mg/kg<br>- Doses per time period: single<br>- Volume administered or concentration: undiluted<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Clinical signs and mortality several times during day 1 after dosing and daily thereafter. Survivors were weighed at the end of the observation period. All animals were subjected to gross necropsy. |
| **Test substance:** | Tradename Isalchem 145 C14-16 alcohols Type A |
| **Conclusion:** | The rat oral LD50 for Isalchem 145 was >5000 mg/kg. There were no clinical signs of intoxication and findings at gross autopsy were unremarkable. |
| **Reliability:** | (2) valid with restrictions<br>Comparable to guideline study with acceptable restrictions. |
| **Flag:** | Critical study for SIDS endpoint |

25-JUL-2005 (8)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 8
**Vehicle:** other: undiluted
**Doses:** 10000 mg/kg
**Value:** > 10000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died

CLINICAL SIGNS: No signs of intoxication

NECROPSY FINDINGS: Not carried out.
**Test condition:** TEST ORGANISMS: Rat Wistar
- Source: Shell Toxicology Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F fasted
- Controls: no

ADMINISTRATION:
- Doses: 12.2 ml/kg (10 g/kg)
- Doses per time period: single dose
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality. No necropsy was carried out.
**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A
**Conclusion:** The rat oral LD50 for Dobanol 45 is > 10,000 mg/kg, there were no clinical signs of toxicity.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (18) (25)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Doses:** 2.9, 3.46, 4.16 and 5 g/kg
**Value:** > 5000 mg/kg bw

**Method:** other:screening test
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** The rat oral LD50 for Lial 145 is >5000 mg/kg. There were no deaths at this dose level.

**Source:** Biolab SGS 1984
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: no data
- Group size: 5M+5F

ADMINISTRATION: Gavage
- Doses: 2.9, 3.46, 4.16 and 5 g/kg
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Mortality
**Test substance:** Tradename Lial 145 C14-16 alcohols Type A
**Reliability:** (4) not assignable
Few study details, screen only.
25-JUL-2005 (5)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 20
**Vehicle:** no data
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other: in house protocol
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died.

CLINICAL SIGNS: No signs of intoxication, no adverse effect on weight gain.

NECROPSY FINDINGS: None reported.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan, Correzzana, Milan, Italy
- Weight at study initiation: 200 g (+- 20g)
- Group size: 5M+5F fasted.
- Controls: Yes

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: not reported
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs and mortality several times during day 1 after dosing and daily thereafter. Survivors were weighed at the end of the observation period. All animals were subjected to gross necropsy.
**Test substance:** Tradename Alchem 145 C14-16 alcohols Type A
**Conclusion:** The acute oral LD50 for Alchem 125 is >5000 mg/kg, there were

no signs of intoxication.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (14)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12 (1-dodecanol), C12-16, C14 (tetradecanol) and C16 (hexadecanol) alcohols in support of the statement that C14-16 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (28) (32)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 8
**Vehicle:** other: undiluted
**Doses:** 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No animals died

CLINICAL SIGNS: No signs of intoxication

NECROPSY FINDINGS: Not carried out.
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall), Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F
- Controls: No

ADMINISTRATION: 24 hour occluded dermal application
- Area covered: not reported applied to shorn dorsolumbar

skin.
- Occlusion: aluminium foil and waterproof plaster.
- Vehicle: undiluted
- Total volume applied: 2.4 ml/kg (2 g/kg)
- Doses: 2.4 ml/kg
- Removal of test substance: washed with tepid dilute detergent solution.

EXAMINATIONS: Mortality and clinical signs during the 14 day observation period.

**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A

**Conclusion:** The rat dermal LD50 for Dobanol 45 is >2000 mg/kg, there were no clinical signs of toxicity.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (18) (25)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Result:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 5 rabbits gave a score of 0.3, the remaining rabbit gave a score of 0.7 (group mean 24+48 +72 hour score 0.4)
- Oedema: Individual 24+48+72 hour scores 5 rabbits gave a scores of 0.3, the remaining rabbit gave a score of 0.7 (group mean 24+48 +72 hour score 0.4)

REVERSIBILITY: All scores were 0 from 72 hours to the end of the observation period.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS 1991d

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Alchem 145 C14-16 alcohols Type A

**Conclusion:** Following a 4 hour occlusive exposure Alchem 145 was not irritating to rabbit skin when assessed by either EU or GHS criteria. All scores <1.5.

**Reliability:** (2) valid with restrictions
Guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

04-JAN-2006 (9)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 3 rabbits scored 0, 2 rabbits 1, 1 rabbit 0.7 (Group mean 24+48+72 hour score 0.44)
- Edema: Individual 24+48+72 hour scores 2 rabbits scored 0, 4 rabbits 0.7 (Group mean 24+48+72 hour score 0.45)

REVERSIBILITY: All scores were 0 from day 5 to the end of the observation period (day 7).

OTHER EFFECTS: None reported

**Source:** Biolab SGS 1991e

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Isalchem 145 C14-16 alcohols Type A

**Conclusion:** Following a 4 hour occlusive exposure Isalchem 145 was not irritating to rabbit skin when assessed by either EU or GHS criteria. All scores <1.5.

**Reliability:** (2) valid with restrictions
Guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (10)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1985
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE

Individual scores not reported.
- Erythema: Group mean 24+48+72 hour score 1.8
- Edema: Group mean 24+48+72 hour score 1.6

REVERSIBILITY: The irritation persisted until the end of the observation period. Group mean 7 day scores were 1.6 for erythema and 1 for oedema.

OTHER EFFECTS: None reported

**Source:** Biolab SGS, 1985c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White

- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml or 0.5g
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 30 mins, 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Lial 145 C14-16 alcohols Type A
**Conclusion:** Following a 4 hour occluded exposure and in the absence of individual scores Lial 145 is at least a mild irritant according to GHS criteria.
**Reliability:** (2) valid with restrictions
Guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (12)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 3
**PDII:** 2.9
**Result:** irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE mean 24+72 hour score
- Erythema: abraded skin - individual 1, 2, 1.8 group mean 1.6 intact skin - individual 1.3, 2, 2 group mean 1.8
- Edema: abraded skin -individual 0.8, 1,5, 1.5 group mean 1.3

REVERSIBILITY: At the end of the 7 days observation period the skin lesions had not regressed, at all test sites the skin was thickened and lifting and cracking slightly. Erythema and oedema scores at 7 days for both intact and abraded skin were 1.5 and 1.7 respectively.
**Source:** Cassidy, 1978d
**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: female
- Source: Shell Toxicology Breeding Laboratory, Sittingbourne, UK

- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2x2 cm
- Occlusion: occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 24 hours to intact and abraded skin.
- Postexposure period: 7 days
- Removal of test substance: Washed with warm dilute detergent solution.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours and at 7 days.

**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A

**Conclusion:** Based on erythema and oedema scores Dobanol 45 might be considered a mild irritant according to GHS criteria. However the degree of irritation showed little evidence of regression by the end of the 7 days observation period and the skin was cracking and lifting, this material is therefore considered irritant to the skin.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (18) (25)

## 5.2.2 Eye Irritation

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual scores 4 rabbits 0.7, 2 rabbits 1 (group mean score 0.7)
- Conjunctivae (Chemosis): Individual scores 4 rabbits 0.7, 2 rabbits 0 (group mean score 0.4)

DESCRIPTION OF LESIONS: Redness (grades 1 and 2) and chemosis (grade 1) were observed in the conjunctivae of all eyes 1 hour after instillation.

REVERSIBILITY: All scores 0 by day 7.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS Undated (b)
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Lial 145 C14-16 alcohols Type A

**Conclusion:** Lial 145 is not classifiable as a eye irritant by either GHS or EU criteria.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (13)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Result:** not irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0.4
- Conjunctivae (Chemosis): 0

individual scores were not reported.

REVERSIBILITY: All eyes were normal at day 7.

OTHER EFFECTS: None reported.

**Source:** Cassidy, 1978d

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: not reported
- Source: Shell Toxicology Laboratory (Tunstall) Breeding

Unit.
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Untreated eye
ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.2 ml
- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: not reported
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: Not reported

**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A
**Conclusion:** Dobanol 45 is not rritating to the eye according to EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (18) (25)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual scores 5 rabbits 0, 1 rabbit 0.7 (group mean score (0.11)
- Conjunctivae (Chemosis): Individual scores 0, 1, 1, 1, 0.7, 0.7 (group mean score 0.7)

DESCRIPTION OF LESIONS: Conjunctival redness (mostly grade 1, 1 animal grade 2) was observed in all eyes and chemosis in 5/6 (one grade 2, 4 grade 1) eyes 1 hour after instillation.

REVERSIBILITY: All eyes scored 0 by day 7. Chemosis persisted in 3 animals to 72 hours.

OTHER EFFECTS: None reported.
**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6

- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Alchem 145 C14-16 alcohols Type A
**Conclusion:** Alchem 145 is not an eye irritant when classified using EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (6)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): Individual scores 5 rabbits 0, 1 rabbit 0.7 (group mean score 0.11)
- Conjunctivae (Chemosis): 0

DESCRIPTION OF LESIONS: All animals showed conjuctival redness and chemosis 1 hour after instillation. (all grade 1 except grade 2 redness in one test eye)

REVERSIBILITY: All scores 0 by 48 hours after instillation.

OTHER EFFECTS: None reported

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None

- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Isalchem 145 C14-16 alcohols Type A
**Conclusion:** Isalchem 145 is not an eye irritant when classified using EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (7)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** other: Hartley albino guinea pigs
**Concentration 1st:** Induction intracutaneous
**2nd:** Induction occlusive epicutaneous
**3rd:** Challenge occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: liquid paraffin
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: Magnusson & Kligman maximization test
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There was no evidence of sensitisation in any of the test animals at any observation point after challenge. Response at 24, 48 and 72 hours 0/20 treated, control response not reported.
**Source:** Biolab SGS, Undated
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Guinea pig
- Strain: Hartley
- Sex:
- Source: Padre Antonio Mariano Comense, Italy
- Age: 250-300g
- Number of animals: 20
- Controls: 10

ADMINISTRATION/EXPOSURE
A general desription of the test procedure was provided without detail of induction and challenge concentrations. Oil soluble or insoluble materials such as Lial 145 are dissolved or suspended in paraffin oil. The animals received intradermal challenge injections with and without Frends Adjuvant on day 1. 6 days later the animals receive a topical application of sodium laruyl sulphate in petrolatum to produce mild irritation. The following day the product is applied under an occlusive patch for 48 hours. Challenge is carried out on day 21 (two weeks after the topical induction) using a topical occlusive 24 hour exposure.

EXAMINATIONS
- Grading system: normal skin =0; faint pink =1; pink,

moderate oedema =2; bright pink, markedly thickened =3.
- Pilot study: no details reported.

**Test substance:** Tradename Lial 145 C14-16 alcohols Type A

**Conclusion:** Lial 145 is not a skin sensitiser when tested using the guinea pig maximization procedure of Magnusson & Kligman.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

05-DEC-2005 (11)

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction 1 % intracutaneous
**2nd:** Induction 50 % occlusive epicutaneous
**3rd:** Challenge 25 % occlusive epicutaneous
**No. of Animals:** 30
**Vehicle:** other: corn oil
**Result:** not sensitizing

**Method:** other: Magnusson & Kligman
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: Not reported

RESULTS OF TEST
- Sensitization reaction: negative, no animals responded.
Response 0/20 test, 0/10 controls at 24 or 48 hours.
- Clinical signs: None
- Rechallenge: None

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: P-strain
- Sex: male & female
- Source: Shell Toxicology Lab (Tunstall) breeding unit.
- Age/weight: Not reported
- Number of animals: 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: Maximization (M&K)
- Preparation of test substance for induction: In corn oil
- Preparation of test substance for challenge: In corn oil
- Induction schedule: Intradermal injection followed one week later by topical application (48 hour occlusive).
- Concentrations used for induction: 1% intradermal, 50% topical (48 hour occlusive).
- Concentration in Freuds Complete Adjuvant (FCA): not reported
- Challenge schedule: 2 weeks after topical induction, 24 hour topical challenge.
- Concentrations used for challenge: 25% in corn oil.
- Rechallenge: No
- Positive control: 1:1

EXAMINATIONS
- Grading system: 4 point scale -ve, trace, +ve, ++ve
- Pilot study: Initial irritation screen, no details given.

**Test substance:** C14-16 alcohols CAS RN 68333-80-2 (Dobanol 45)

**Conclusion:** Dobanol 45 is not a skin sensitiser when tested according to

the guinea pig maximization assay.

This study is reported in iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

05-DEC-2005 (18) (25)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-chronic
**Species:** rat **Sex:** male/female
**Strain:** Wistar
**Route of administration:** oral feed
**Exposure period:** 90 days
**Frequency of treatment:** continuously
**Post exposure period:** none
**Doses:** 0, 0.2, 1.0, and 5.0%
**Control Group:** yes
**NOAEL:** = 167 mg/kg bw
**LOAEL:** = 736 mg/kg bw

**Method:** other: see text
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** NOAEL: 0.2% (ca 200 mg/kg/day)

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: The dose levels were based on the results of a 14 day preliminary study in which groups of rats received 0.5, 1, 3 and 10% Dobanol 45 in the diet. As only the 10% level showed any fatalities or signs of intoxiciation the dose levels for the 90 day study were set at 0.2, 1 and 5% in the diet. These are equivalent to:
Mean intake mg/kg/day: 0.2% M 171 (101-317) F 167 108-271); 1% M 759 (488-1301); 5% M 3626 (2660-5659) F 3491 (2529-4802)

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No animals died during the study.
- Clinical signs: Unremarkable
- Body weight gain: At the low dose level (0.2%) body weights were similar between treated and control groups.
Administration of 1 or 5% in the diet resulted in reduced weight gain which reached statistical significance from 1-3 weeks after exposure commenced to the end of the study.
- Food/water consumption: These followed a similar trend with the 2 higher dose levels showing reduced food and water intake, food loss due to spillage was frequently reported in these groups. Food efficiency was incresed in mid and top dose males and females for most of the exposure period.
- Clinical chemistry: Significant changes from control are as shown below:

| Dose Males | AP (KA-U) | ALAT (K-U) | T-P (g/dl) | A/G mg/dl | T-chol mEq l | K- |
|---|---|---|---|---|---|---|
| Control | 13.0 | 37.7 | 5.79 | 1.12 | 39.5 | 4.45 |
| 0.2% | 13.7 | 46.0 | 5.93 | 1.09 | 40.5 | 4.66 |
| 1% | 15.6** | 36.5 | 5.94* | 1.14 | 43.0 | 4.66 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 5% | 16.4** | 71.6** | 5.52* | 1.25** | 42.2 | 4.93** |
| Females | | | | | | |
| Control | 12.9 | 35.3 | 5.78 | 1.12 | 52.1 | 4.45 |
| 0.2% | 12.4 | 36.7 | 5.83 | 1.12 | 52.8 | 4.36 |
| 1% | 15.5** | 35.8 | 5.75 | 1.13 | 52.6 | 4.27 |
| 5% | 19.8** | 99.4** | 5.55* | 1.28** | 42.7** | 4.38 |

- Haematology: Hb was significantly reduced (at 1% level) in top dose males 15.2 g/dl (+-0.5) compared to 15.9 (+-0.4) for controls. Eosinophils were significantly reduced at all dose levels in males but this was not dose related (control 1.5%; low dose 0.6%; mid dose 0.2%; high dose 0.6%). In females the only significant change (1% level) was increased WBC in top dose animals (control 100/mm3 47 (+- 12.2) top dose 73.2 (+-16.2). This was not accompanied by any significant changes in the differential leucocyte count. There was no increase in WBC at the low and mid dose mean values being 45.2 and 45.5 respectively.
- Urinalysis: No treatment related changes.
- Organ weights: The more significant changes (either seen in both sexes or dose related) in relative organ weights expressed in mg/100g (thyroid & adrenal) or g/100g are shown in the table below.

| Dose | Brain | Thyroid | Testes | Liver | Kidney | Adrenal |
|---|---|---|---|---|---|---|
| Males | | | | | | |
| Control | 0.57 | 4.55 | 0.91 | 3.14 | 0.61 | 11.6 |
| 0.2% | 0.57 | 4.72 | 0.90 | 3.09 | 0.59 | 12.3 |
| 1% | 0.61** | 5.07* | 0.98* | 3.30 | 0.62 | 13.0* |
| 5% | 0.71** | 5.53** | 1.12** | 4.08** | 0.71* | 15.4** |
| Females | | | Ovary | | | |
| Control | 0.93 | 6.05 | 31.8 | 2.89 | 0.61 | 26.1 |
| 0.2% | 0.92 | 6.52 | 31.0 | 2.98 | 0.64 | 24.8 |
| 1% | 0.96 | 6.79 | 32.0 | 3.12* | 0.65** | 26.0 |
| 5% | 0.96 | 7.60** | 36.8** | 3.97** | 0.70** | 25.9 |

Absolute organ weights also showed significant changes as follows: At 5% for both sexes brain & heart weight were decreased. Relative heart wt. was slightly increased in males only. Absolute and relative lung weights were incresed in males but not females. Absolute thymus weight was decreased in top dose males. Absolute liver, kidney. and thyroid weights were increased in top dose females, while absolute kidney and spleen weights were increased in top and mid dose males. None of the changes in organ weight were accompanied by histopathological change. No biologically signficant changes in either absolute or relative organ weights were observed at the low dose level (0.2%).

- Gross pathology: Blood was observed in the stomach of 1 female in each of the mid and high dose groups. There were no other remarkable changes.
- Histopathology: There were no treatment related changes. Slight kidney changes such as hyaline casts, calculi and increased medullary connective tissue were observed but these were not dose related. In the liver there were no histopathological changes in mid and high dose groups. At 0.2% slight focal necrosis was observed in 1/5 females examined. No abnormalites were observed in any other organs including the gonads.

**Source:** Ito 1978.

Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS
- Age: 5 weeks
- Number of animals: 11M+11F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 90 days
- Type of exposure: dietary
- Post exposure period: none
- Vehicle: diet
- Concentration in diet: 0, 0.2, 1 and 5%

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Twice weekly
- Food consumption/food efficiency: Twice weekly
- Water consumption: Weekly
- Ophthalmoscopic examination: Not done
- Haematology: RBC, Hb, Haemocrit, platelet count, WBC and differential count.
- Biochemistry: Alkaline phosphatase, ALAT, ASAT, total cholesterol, urea nitrogen, Na, K.
- Urinalysis: pH, protein, sugar, ketone bodies, occult blood at 90 days

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: general examination
- Organ weights: brain, hypophysis, thyroid, thymus, heart, liver, kidney, spleen, adrenal, testes or ovaries.
- Microscopic: the above mentioned organs plus stomach, pancreas, small & large intestine, lymph gland, bone marrow.

STATISTICAL METHODS: Student t test.

**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A

**Conclusion:** NOAEL 0.2% equivalent to a mean dose of 171 mg/kg/day in males and 167 mg/kg/day in females. LOAEL 1% (M 759 mg/kg/day F 736 mg/kg/day). Effects seen at higher dose levels are inhibition of body weight gain probably due to decreased food consumption. Increases in liver weight were associated with increased liver enzyme actiivity (alkaline phosphatase and ALAT) but not with histopathological change . The increase in food efficiency seen at the higher dose levels is considered indicative that the restriction in body weight is due to unpalatability rather than a toxic effect of the test material and may be a confounding factor in the changes in liver enzyme levels.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (24)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro

testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C14-16 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol and hexadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (28) (32)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol, dodecanol, C12-16 (types A & B), C12-18 (type B), tetradecanol, hexadecanol and octadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (23) (28) (29) (32)

## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

**Type:** other: Repeat dose study with histopathology of reproductive organs.

**Species:** rat

**Sex:** male/female

**Strain:** Wistar

**Route of administration:** oral feed

**Exposure Period:** 90 days

**Frequency of treatment:** continuously
**Doses:** 0, 0.2, 1.0, and 5.0%
**Control Group:** yes
**NOAEL Parental:** = .2 %

**Method:** other: The test substance was mixed into the feed of male and female rats at the different doses. The animals were observed throughout the 90 period. Urine and blood were analyzed along with internal organs.
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were increases in both testes and ovary weights ($p<0.1$) at the top dose level of 5% (ca 3500 mg/kg/day). Testes weight was also increased at the 1% dose level ($p<0.05$). No histopathological changes were reported in the gonads at any dose level. The NOAEL for systemic toxicity and effects on the reproductive organs is 0.2% in the diet (ca 200 mg/kg/day) (males 171 mg/kg/day; Females 167 mg/kg/day).
**Source:** Ito 1978.
Hayes Consultancy Service Bromley, Kent
**Test condition:** Rats received Dobanol 45 in the diet for 90 days at dose levels of 0, 0.2, 1 and 5%. The usual parameters were investigated and full details of the study are to be found in Chapter 5.4 Repeat dose toxicity. Both testes and ovaries were weighed and examined histopathologically.
**Test substance:** Tradename Dobanol 45 C14-16 alcohols Type A
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (24)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C14-16 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (28) (29) (32)

**5.8.3 Toxicity to Reproduction, Other Studies**

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**5.9 Specific Investigations**

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**5.10 Exposure Experience**

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**5.11 Additional Remarks**

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(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(5) Biolab SGS 1984 Acute oral toxicity Lial 145 (CAs no 68333-80-2) Protocol no 1205 dated 27.3.84

(6) Biolab SGS 1991i Acute eye irritation. Alchem 145 protocol no. 5683/5 dated 28.10.91

(7) Biolab SGS 1991j Acute eye irritation. Isalchem 145 protocol 5683/2 dated 28.01.91

(8) Biolab SGS. 1990b. Acute oral toxicity Isalchem 145.

(9) Biolab SGS. 1991d. Primary skin irritation Alchem 145. Protocol No. 5683/5 summary report dated 28.01.91.

(10) Biolab SGS. 1991e. Primary skin irritation Isalchem 145. Protocol No. 5683/2 summary report dated 28.01.91.

(11) Biolab SGS. Undated. CAS No. 68333-80-2 Lial 145. Allergic skin sensitization. Report No. 3008.

(12) Biolab SGS. 1985c. Primary skin irritation Lial 145. Protocol No. 4954 summary report dated 1985

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(29) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

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Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(33) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 68603-15-6 |
| **CAS No.** | 68603-15-6 |
| **EINECS Name** | Alcohols, C6-12 |
| **EC No.** | 271-642-9 |
| **TSCA Name** | Alcohols, C6-12 |

| | |
|---|---|
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |

| | |
|---|---|
| **Printing date:** | 10-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **18-JAN-2006** |

| | |
|---|---|
| **Number of Pages:** | **80** |

| | |
|---|---|
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

04-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
11-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C6-12 alcohols, CAS 68603-15-6 are 5-100% linear.

The substance comprises C6-12 alcohols. Components of even or even and odd chain length, in the range C6-13 are present.

Commercial products marketed under this CAS number fall into four types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A, Type B, Type C and Type D.

Type A products are 5-95% linear. The substance comprises >= 95% C11. Components of even and odd chain length, in the range C9-C13 are present.

Type B products are >80% linear. The substance comprises > 95% C9, 10 and 11. Components of even and odd chain length, in the range C8-C12 are present.

Type C products are >80% linear. The substance comprises > 95% C7, 8 and 9. Components of even and odd chain length, in the range C6-C10 are present.

Type D products are 100% linear. The substance comprises >=90% C8 and 10; <10% C6. Components of even chain length, in the range C6-C12 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Alcohols, C6-12 (CA INDEX NAME)
Alcs., C6-12
Alcs., fatty C6-12
C6-12 alcohols
C6-12 alcs.

Fair 85
Off-Shoot T

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C6-12 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 000 - 25 000 tonnes (CAS-specific data) - This is

the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 000 - 50 000 000 pounds.

21-DEC-2005 (4) (23) (42)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available
19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Surface Treatment
19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 125, 165, 71 and 1482
05-AUG-2005 (44)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C6-12 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
04-AUG-2005

## 2.1 Melting Point

**Value:** = -16 - -4 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-SEP-2005 (35)

## 2.2 Boiling Point

**Value:** = 180 - 214 degree C at 1013 hPa
**Decomposition:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-SEP-2005 (21)

## 2.3 Density

**Value:** = .83 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
05-OCT-2005 (21)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** It is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (39)

### 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0044 - .17 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.0044 hPa
Type B: 0.013 hPa
Type C: 0.17 hPa
Type D: 0.16 hPa
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
05-OCT-2005 (1)

**Value:** < .04 hPa at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
05-OCT-2005 (21)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 2.3 - 4.2
**PH prec:** = 6.7

**Method:** other (measured)
**Year:** 1984
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The log n-octanol/water partition coefficient was determined by reverse-phase HPLC and by the fragment-addition method.
**Result:** Log Kow was determined by reverse-phase HPLC and by the fragment-addition method to be 2.3-4.2 and 2.5-3.5 respectively.
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (25)

**log Pow:** = 4.6 - 6.4 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of Ph (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

**Result:** Type A: ca. 4.7
Type B: 3.8 - 4.7
Type C: 2.6 - 3.8
Type D: 2.0 - 4.6

**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.

**Flag:** Critical study for SIDS endpoint

15-SEP-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 9.7 - 510 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 9.7 mg/l at a loading rate of 1000 mg/l
Type B: 43.9 mg/l at a loading rate of 1000 mg/l
Type C: 510 mg/l at a loading rate of 1000 mg/l
Type D: 293 mg/l at a loading rate of 1000 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

15-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 79 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
05-OCT-2005 (21)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
18-JAN-2006 (3)

**Type:** air
**Light source:** Sun light
**Conc. of subst.:** at 20 degree C
**INDIRECT PHOTOLYSIS**
**Sensitizer:** OH
**Conc. of sens.:** 1000000 molecule/$cm^3$
**Rate constant:** = .000000000013358 $cm^3$/(molecule * sec)
**Degradation:** = 50 % after .8 day(s)

**Method:** OECD Guide-line draft "Photochemical Oxidative Degradation in the Atmosphere"
**Year:** 1990
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.
**Flag:** Critical study for SIDS endpoint
18-JAN-2006 (20)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4.However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** Type A:
TGD Hydrophobics method: Koc = CA. 7270
TGD Non-hydrophobics method: Koc = ca. 3000
TGD Alcohols method: Koc = ca. 220
SRC PCKOCWIN method: Koc = ca. 180

Type B:
TGD Hydrophobics method: Koc = 1430 - 8380
TGD Non-hydrophobics method: Koc = 960 - 3000
TGD Alcohols method: Koc = 90 - 220

SRC PCKOCWIN method: Koc = 50 - 180

Type C:
TGD Hydrophobics method: Koc = 152 - 1430
TGD Non-hydrophobics method: Koc = 230 - 960
TGD Alcohols method: Koc = 30 - 90
SRC PCKOCWIN method: Koc = 15 - 50

Type D:
TGD Hydrophobics method: Koc = 56 - 6330
TGD Non-hydrophobics method: Koc = 450 - 2500
TGD Alcohols method: Koc = 50 - 190
SRC PCKOCWIN method: Koc = 30 - 100

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only for the upper limit of the range.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

29-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** predominantly domestic sewage
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 64 - 79 % after 28 day(s)
**Result:** readily biodegradable
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test substance was added to the test medium from a stock solution containing 2.4 g/l test substance emulsified in Dobane PT sulphonate. The test medium was dispensed into the Sturm vessels, inoculated and aerated with 60 ml/min of CO2-free air. The extent of biodegradation at 2, 6, 9, 12, 19 and 28 days was determined by titrating the total carbon dioxide released from the incubation. The medium was acidified on day 27 to release the total carbon dioxide by day 28.
**Remark:** The following validity criteria were fulfilled (1) the reference substance reached the pass level by day 14; (2) parallel assays did not differ by greater than 20%.
**Result:** The test substance degraded >60% during the '10-day window' in the Modified Sturm test. The reference substance, Sodium benzoate, degraded by 77% after 28 days.
**Test condition:** Concentration of inoculum: not reported
Test volume: not reported

Temperature: not reported
pH: not reported
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (22)

**Type:** aerobic
**Inoculum:** predominantly domestic sewage
**Concentration:** 2 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 53 - 54 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 5 day(s) = 38 %
15 day(s) = 54 %
28 day(s) = 54 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test substance was added to the test medium from a stock solution containing 2.4 g/l test substance emulsified in Dobane PT sulphonate. The final test concentration was 2 mg/l test substance. The bottles were incubated at 21 ± 1°C and the extent of biodegradation at 5,15 and 28 days was determined by measuring the oxygen concentration in the bottles.
**Remark:** The following validity criteria were fulfilled:
(1) oxygen uptake in the inoculum blank did not exceed 1.5 mg/l after 28 days;
(2) dissolved oxygen concentrations did not fall below 0.5 mg/l;
(3) the reference substance reached the pass level by Day 14;
(4) parallel assays did not differ by greater than 20%;
(5) the toxicity control attained > 25% degradation in 14 days.
**Result:** Kinetic of control substance:
5 days = 60%
15 days = 62%
28 days = 71%
The test substance degraded < 60% over the test period, therefore cannot be considered readily biodegradable.
**Test condition:** Concentration of inoculum: not reported
Test volume: not reported
Temperature: 21 ± 1°C
pH: not reported
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
17-OCT-2005 (22)

**Type:** aerobic
**Inoculum:** other: settled sewage - origin unknown
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 79 % after 28 day(s)
**Result:** readily biodegradable

**Method:** other: modification of the Sturm-Weaver test procedure
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A modification of the Sturm Weaver test was performed. 6% CaCl2 on DOBS PT active matter is added to stabilise the emulsion. Carbon dioxide-free air is passed through the solution. The carbon dioxide evolved during biodegradation is carried to barium hydroxide absorbers by the air stream. Comparing the titration with hydrochloric acid to a phenolphthalein endpoint for the product against that for the blank allows the mass of carbon dioxide evolved to be calculated. The test is continued until plateau conditions are obtained, normally 26-30 days. This method corresponds to OECD 301B, except that the inoculum was taken from an acclimated culture.
**Remark:** No information is provided on the validity criteria of the study.
**Result:** 11 days = 62%
15 days = 67%
21 days = 72%
26 days = 77%
28 days = 79%
The test substance degraded >60% within the 10 day window.
**Test condition:** Inoculum concentration: A 10% solution of settled sewage in BOD water containing 20 mg/l of product and 50 mg/l of soluble yeast extract was allowed to stand quiescently in the dark for 14 days. The supernatant liquid was used as inoculum.
Test volume: not reported
Temperature: not reported
pH: not reported
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (3) invalid
Study was considered invalid due to significant methodological deficiencies, inoculum was acclimated before use.
17-OCT-2005 (41)

**Type:** aerobic
**Inoculum:** other: no details provided on the inoculum
**Concentration:** 38 mg/l related to Test substance
**Contact time:** 37 day(s)
**Degradation:** = 83 % after 26 day(s)
**Result:** readily biodegradable

**Method:** other: OECD 301F and ISO 9408
**Year:** 1993
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The following validity criteria were met (1) The oxygen uptake of the inoculum blank was less than 60 mg/l over 28 days, (2) Parallel assays did not differ by more than 20%, (3) reference compound reached the pass level within 14 days. No information was provided on the pH of test system.
Kinetic of test substance:
1 days = 17%
8 days = 66%
26 days = 83%
30 days = 84%
37 days = 85%
Control substance: Sodium benzoate
Kinetic of control substance:
1 days = 44%
8 days = 83%
26 days = 90%
30 days = 93%
37 days = 91%
**Result:** The substance degraded >60% within the 10 day window, therefore it is considered readily biodegradable.
**Test condition:** Inoculum concentration: not reported
Temperature: not reported
pH: not reported
Test volume: 500 ml
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Guideline study conducted to GLP but some experimental details not reported.
**Flag:** Critical study for SIDS endpoint
17-OCT-2005 (19)

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to all compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (14)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 10 - 2050

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Result:** Type A: BCF estimated as 1800 - 2050
Type B: BCF estimated as 320 - 2050
Type C: BCF estimated as 30 - 320
Type D: BCF estimated as 10 - 1530

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Idus idus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = .7 - .8
**Limit Test:** no

**Method:** other: Fischtest L15
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
96 hr LC50 = 0.7 - 0.8 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

No deaths were observed at 0.7 mg/l during 96 hours, while 0.8 mg/l killed all exposed fish in 24 hours. Only a toxicity range could be quoted owing to the steepness of the log dose-response curve.
**Source:** Reiff 1978
**Test condition:** TEST ORGANISMS
Strain: idus idus melanotus
Supplier: Imported from Germany by Messrs CURA of Hemel Hempstead, Herts, UK
Age: not reported
Weight: 2.1 g average
Feeding: not reported
Pretreatment: not reported
Feeding during test: not reported
Control group: 1 control group (5 fish)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle, solvent: 400 mg/l
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Dechlorinated mains water
Aeration: Continuous gentle aeration
Alkalinity: not reported
Hardness: 260 mg/l as CaCO3
Conductance: not reported
TEST SYSTEM
Concentrations: 0.5, 0.6, 0.7, 0.8 and 1.0 mg/l
Exposure vessel type: All-glass aquaria
Number of replicates: 1
Fish per replicate: 5
Test temperature: 20 C
Dissolved oxygen: > 7 mg/l
pH mean: 8.2 - 8.4
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported

TEST PARAMETER: mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: none

**Test substance:** This result was measured for a commercial product of compositional Type C.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (29)

**Type:** semistatic
**Species:** other: Juvenile turbot (Scophthalmus maximus)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 5.8
**Limit Test:** no

**Method:** other
**Year:** 1991
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Due to only partial mortality being achieved at 5.6 mg/l an extra exposure level of 10 mg/l was added to the test series at 72 hours, with 100% mortality being achieved within 3 hours. Mortality data from the 10 mg/l exposure level was included in the statistical analysis.

**Result:** RESULTS: EXPOSED
24hr LC50 = 6.7 mg/l
48hr LC50 = 6.3 mg/l
96hr LC50 = 5.8 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Huntingdon Life Sciences Ltd 1991d.

**Test condition:** TEST ORGANISMS
Strain: Juvenile Turbot (Scophthalmus maximus)
Supplier: Golden Sea Produce Ltd., Hunterston, Scotland
Weight: 3.17 g
Feeding: Commercial pellets
Pretreatment: Acclimatised 10 days prior to start of test
Feeding during test: Not reported
Control group: 1 control and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: 1% Tween 80-acetone
Concentration of vehicle, solvent: Not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Synthetic sea water (Synthetica) at 32% S
Aeration: At least 12 hours prior to use by propeller-stirrers
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 0.56, 1.0, 1.8, 3.2, 5.6 and 10 mg/l
Exposure vessel type: Glass aquaria
Number of replicates: 1
Fish per replicate: 10
Test temperature: 14 +/- 1 C
Dissolved oxygen: >= 7.9 mg/l

pH mean: not reported
Photoperiod: 16 h light : 8 h dark
TEST PARAMETER: mortality
SAMPLING: Mortality was recorded at 3, 6, 24, 48, 72 and hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (18)

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 6.3 - 10
**Limit Test:** no

**Method:** other
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Five fish were placed in each of six all-glass aquaria containing 10 l of dechlorinated mains water. Quantities of a 100 mg/l solution of Dobanol 91 in acetone had previously been added to the water to give a series of approximately logarithmically graded concentrations.
**Source:** Shell Toxicology Laboratory 1979
**Test substance:** Test substance freetext: This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with same reliability score and showing greater toxicity are available.
11-OCT-2005 (33)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 1.7 - 13

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The range of results given above reflects variable composition

between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 1.7 mg/l;
Type B: 2.1 mg/l;
Type C: 13 mg/l;
Type D: 3.8 mg/l;

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

30-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** semistatic
**Species:** Crangon crangon (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 4.6
**Limit Test:** no

**Method:** other
**Year:** 1991
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test animals were slightly smaller than the range quoted in the protocol (4-6 cm) due to seasonal availability but this was not considered to have had a significant effect on the results of the test.

**Result:** RESULTS: EXPOSED
24 hr LC50 = 6.6 mg/l
48 hr LC50 = 5.6 mg/l
96 hr LC50 = 4.6 mg/l
Based on nominal concentrations
RESULTS:
CONTROL
Number/% showing adverse effects: 1
SOLVENT CONTROL
Number/% showing adverse effects: 1

**Source:** Huntingdon Life Sciences Ltd 1991a.

**Test condition:** TEST ORGANISMS
Strain: Crangon crangon
Supplier: P. Garnett, King's Lynn, Norfolk
Weight: 1.46 g
Feeding: None
Pretreatment: Acclimatised 6 days prior to test
Feeding during test: Not reported
Control group: 1 control and 1 solvent control group (100 ul/L)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: 1% Tween 80-acetone
Concentration of vehicle, solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Synthetic sea water (Synthetica) at 32% S

Aeration: At least 12 hours prior to use by propeller-stirrer
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: 1, 1.8, 3.2, 5.6 and 10 mg/l
Renewal of test solution: Daily
Exposure vessel type: Glass aquaria
Number of replicates: 1
Invertebrate per replicate: 20
Test temperature: 14 +/- 1C
Dissolved oxygen: >= 7.9 mg/l
pH mean: not reported
Adjustment of pH: Not reported
Intensity of irradiation: Not reported
Photoperiod: 16 h light : 8 h dark
TEST PARAMETER: Mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

21-OCT-2005 (17)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EC50:** = 5.9
**EC10 :** = 1.5
**Limit Test:** no

**Method:** OECD Guide-line 202
**Year:** 2005
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Nature of adverse effects: immobilisation
Based on measured concentrations
0% of control animals died after 24 hours
EC50 5.9 (4.3-8.2) mg/l
NOEC = 1.1 mg/l
LOEC = 3.1 mg/l

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: German Federal Environment Agency
Feeding: Scenedesmus subspicatus
Feeding during test: None
STOCK AND TEST SOLUTION AND THEIR PREPARATION
A stock solution was prepared at a nominal concentration of 400 mg/l and this was serially diluted to prepare nominal test concentrations of 0.92, 2.3, 5.8, 14 and 36 mg/l. The corresponding mean measured concentrations of the substance in the test solutions over the duration of the test were 1.1, 3.1, 6.3, 18 and 41 mg/l.
Vehicle, solvent: none
DILUTION WATER
Source: Purified drinking water that was aerated to saturation.

Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Exposure vessel type: 100 ml glass conical flasks with ground-glass stoppers.
Number of replicates: 4
Invertebrate per replicate: 5
Test temperature: 21 degrees C
Dissolved oxygen: 76-92%
pH mean: 8.6-9.5
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Concentrations of the test substance were measured by GC-MS at the start of the test and then again after 24 and 48 hours.

**Test substance:** This result was measured for a commercial product of compositional Type C.

**Reliability:** (1) valid without restriction
GLP-compliant study, conducted in accordance with the standard test guideline.

**Flag:** Critical study for SIDS endpoint

21-OCT-2005 (45)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 7
**Limit Test:** no

**Method:** other
**Year:** 1983
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** 100 ml of test medium was added to a series of 150 ml glass crystallising dishes. Quantities of stock solutions of the test material were added to triplicate sets of dishes to give a logarithmic series of concentrations covering a suitable range. Three dishes received no test material and served as controls.

**Source:** Garforth, B.M. 1983.

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (2) valid with restrictions
Not key study: Other studies with same reliability score and showing greater toxicity are available.

11-OCT-2005 (16)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 11
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test substance was not wholly soluble at concentrations of 10 mg/l and above. Concentrations were expressed in terms of the quantity initially added.

**Result:** RESULTS: EXPOSED
24 hr LC50 = 14 mg/l
48 hr LC50 = 11 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Pearson and Eadsforth 1984.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: ICI Brixham Laboratory
Age: < 24 hours old
Feeding: Concentrated Chlorella vulgaris and active dried yeast daily
Pretreatment: not reported
Feeding during test: not reported
Control group: Three control flasks
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF THE TEST CHEMICAL SOLUTIONS:
Considered stable
DILUTION WATER
Source: Reconstituted fresh water
Aeration: not reported
Alkalinity: not reported
Hardness: 171 mg/l as CaCO3
Conductance: not reported
TEST SYSTEM
Concentrations: Logarithmic series ranging from 0.1 to 100 mg/l
Renewal of test solution: none
Exposure vessel type: 140 ml glass flasks
Number of replicates: 3
Invertebrate per replicate: 10
Test temperature: 17.5 - 22 C
Dissolved oxygen: 8.9 - 9.0 mg/l
pH mean: 8.1 - 8.3
Adjustment of pH: not reported
Intensity of irradiation:
Photoperiod: not reported
TEST PARAMETER: not reported
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Test substance:** This result was measured for a commercial product of compositional Type C.

**Reliability:** (2) valid with restrictions

21-OCT-2005 (25)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 8.5
**Limit Test:** no

**Method:** other

**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test method used was identical to that used in Garforth 1983.
**Source:** Stephenson 1982a.
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
11-OCT-2005 (40)

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 1.7 - 19

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 1.7 mg/l;
Type B: 2.3 mg/l;
Type C: 19 mg/l;
Type D: 4.3 mg/l;
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
17-OCT-2005 (15)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Selenastrum capricornutum (Algae)
**Endpoint:** biomass
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 3.1
**Limit Test:** no

**Method:** other
**Year:** 1984

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
96 hr LC50 = 3.1 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Pearson and Eadsforth 1984.
**Test condition:** TEST ORGANISMS
Strain: Selenastrum capricornutum
Source/Supplier: American Type Culture Collection, Maryland, USA
Pretreatment: not reported
Controls: 6 flasks served as controls
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS
Considered stable
DILUTION WATER
Source: Standard nutrient medium
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: Logarithmically spaced series of concentrations ranging from 1 to 1000 mg/l
Renewal of test solution: not reported
Exposure vessel type: Erlenmeyer flasks
Number of replicates: 1
Initial cell concentration: 500 cells/ml
Test temperature: 22 - 26 C
Dissolved oxygen: not reported
pH mean: 7.5 -7.8
Adjustment of pH: not reported
Intensity of irradiation: approx. 3000 lux
Photoperiod: Constant illumination
TEST PARAMETER: growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: none
**Test substance:** This result was measured for a commercial product of compositional Type C.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with same reliability score and showing greater toxicity are available.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (25)

**Species:** Selenastrum capricornutum (Algae)
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 1
**EC50:** = 2.7
**Limit Test:** no

**Method:** other
**Year:** 1982
**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
EC50 = 2.7 mg/l
Based on nominal concentrations
**Source:** Stephenson 1982a.
**Test condition:** TEST ORGANISMS
Strain: Selenastrum capricornutum
Supplier: American Type Culture Company, Maryland, USA
Pretreatment: Not reported
Controls: Six replicates with 0.5 ml/L acetone
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: 0.5 ml/L
STABILITY OF TEST CHEMICAL SOLUTIONS
Judged to be stable
DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: 1-43 mg/l
Exposure vessel type: Erlenmeyer flask
Number of replicates: 1
Initial cell concentration: 5000 cells/ml
Test temperature: 24 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: Not reported
Intensity of irradiation: Not reported
Photoperiod: Under constant illumination
TEST PARAMETER: Growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION:
None
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (40)

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. 1 - 10

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, in the same way.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

or Types A and D, for which estimation of algal toxicity is required, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The EC50 values obtained by prediction are:
Type A and D: both 1 - 10 mg/l
Measured data for Types B and C are available and so these are not estimated here.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (15)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

## 4.6.3 Toxicity to Soil Dwelling Organisms

-

## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

**Species:** other: Anas platyrhynchos (duck) and Colinus virginianus (quail)
**Endpoint:** mortality
**Unit:** mg/kg bw
**LD50 :** > 4640

**Method:** other: The birds were given a single oral dose via capsule, then observed for 14 days.
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Office of Pesticide Programs 1995.
**Reliability:** (2) valid with restrictions
11-OCT-2005 (24)

## 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of

hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (13)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | other: CD strain rat (remote Sprague-Dawley origin) |
| **Sex:** | male/female |
| **No. of Animals:** | 10 |
| **Vehicle:** | other: maize oil |
| **Doses:** | 2 g/kg |
| **Value:** | > 2000 mg/kg bw |
| **Method:** | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year:** | 1996 |
| **GLP:** | yes |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: None<br><br>CLINICAL SIGNS: Hunched posture and piloerection were observed in males between 30 minutes and 3 hours after dosing. The animals were fully recovered by day 2. No signs in the females. All animals gained bodyweight over the observation period.<br><br>NECROPSY FINDINGS: No significant macroscopic lesions.<br><br>POTENTIAL TARGET ORGANS: None indicated.<br><br>SEX-SPECIFIC DIFFERENCES: Males may be rather more susceptible as they exhibited some signs of intoxication while females did not. However the females may have been slightly older than the males given that the weight range was similar in both sexes. There were no mortalities in either sex. |
| **Source:** | Shell 1996a<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Rat<br>- Source: Charles River Ltd, Margate, Kent, UK<br>- Age: 5 weeks approx.<br>- Weight at study initiation: males 116-130 g; females 119-130g.<br>- Group size: 10M+10F fasted<br>- Controls: No<br>ADMINISTRATION:<br>- Doses: Limit dose of 2000 mg/kg<br>- Doses per time period: Single administration.<br>- Volume administered or concentration: 10 ml/kg in maize oil<br>- Post dose observation period: 15 days<br><br>EXAMINATIONS: Body weights were recorded on the day prior to dosing and on days 1, 8 and 15. Observations of the animals for clinical signs of intoxication were made several times on |

the day of dosing and then throughout the observation period. All animals were autopsied at the end of the study, larger organs were sectioned and the gastro-intestinal tract opened at intervals for examination of the mucosal surface. There was no histopathological examination.
**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The rat oral LD50 for Linevol 79 is >2 g/kg. Signs of intoxicaton consisted of hunched appearance and piloerection on dosing day. There were no significant macrosopic lesions.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (31)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 8
**Vehicle:** other: undiluted
**Doses:** 10 ml/kg (8.3 g/kg)
**Value:** > 8300 mg/kg bw

**Method:** other: standard in house procedure
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: One male died
- Time of death: day 2

CLINICAL SIGNS: Diarrhoea was the only clinical sign.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: No conclusion
**Source:** Cassidy & Clark, 1978b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat
- Source: Shell Toxicology Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F fasted
- Controls: no

ADMINISTRATION:
- Doses: 10 ml/kg (8.3 g/kg)
- Doses per time period: single dose
- Volume administered or concentration: undiluted
- Post dose observation period: 9 days

EXAMINATIONS: Clinical signs and mortality. No necropsy was carried out.
**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The rat oral LD50 for undiluted Linevol 79 was > 8.3 g/kg.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (12)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: undiluted
**Doses:** 10 ml/kg (8.3 g/kg)
**Value:** > 8300 mg/kg bw

**Method:** other: standard in house procedure
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No rats died.

CLINICAL SIGNS: Diarrhoea was the only clinical sign.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: No conclusion
**Source:** Cassidy and Clark 1978
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat
- Source: Shell Toxicology Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F fasted
- Controls: no

ADMINISTRATION:
- Doses: 10 ml/kg (8.3 g/kg)
- Doses per time period: single dose
- Volume administered or concentration: undiluted
- Post dose observation period: 9 days

EXAMINATIONS: Clinical signs and mortality. No necropsy was carried out.
**Test substance:** Tradename Dobanol 91 Type B
**Conclusion:** The rat oral LD50 for Dobanol 91 was >8.3 g/kg. Diarrhoea was the only clinical sign.

This study was reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (11) (20)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 20
**Vehicle:** other: undiluted
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** other: OECD 1981
**Year:** 1981

**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived to the end of the 14 day observation period.

CLINICAL SIGNS: None observed. There were no adverse effects on bodyweight.

NECROPSY FINDINGS: None reported

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None.

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan-Correzzana, Milan, Italy
- Weight at study initiation: 200g (+- 20 g)
- Group size: 5M+5F
- Controls: yes

ADMINISTRATION: Gavage
- Doses: 5000 mg/kg
- Doses per time period: single (animals fasted)
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Clinical observations made at frequent intervals on the day of dosing then daily. Any decedents and all survivors were necropsied at the end of the observation period. Body weights were recorded at the end of the observation period and compared to controls.

**Test substance:** Tradename Lial 111 Type A
**Conclusion:** The rat oral LD50 for Lial 111 is >5000 mg/kg. There were no signs of toxicity.
**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (7)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 5
**Vehicle:** other: atmosphere generated as a mist
**Doses:** 0.58 mg/l
**Exposure time:** 4 hour(s)
**Value:** > .58 mg/l

**Method:** other: in house protocol
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All rats survived the exposure and subsequent observation period.

CLINICAL SIGNS: During the exposure period 50% of the rats salivated and a red nasal discharge was observed. These signs had disappeared by the following day. Body weight data was not reported.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported.

**Source:** Blair and Sedgwick 1980a
Hayes Consultancy Service Bromley, Kent

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C

**Conclusion:** The rat 4 hour LC50 for a mist of Linevol 79 is >0.58 mg/l. Signs of intoxication were transient and confined to salivation and red nasal discharge in some rats during exposure.

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit, Sittingbourne, Kent, UK
- Age: 11 weeks approx.
- Weight at study initiation: not reported
- Number of animals: 5M+5F
- Controls: none

ADMINISTRATION:
- Type of exposure: 4 hour inhalation exposure, whole body
- Concentrations: 0.58 mg/l (atmosphere analysed gravimetrically throughout exposure at 30 minute intervals).
- Particle size: 3.4 um (geometric standard deviation 1.5)
- Type or preparation of particles: mist

EXAMINATIONS: Clinical signs observed throughout exposure and daily thereafter throughout the 14 day observation period. Initial and terminal bodyweights were recorded.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions, not carried out to GLP but subject to QA audit.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (9)

**Type:** LC50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: vapours
**Doses:** 237 mg/l (near saturated atmosphere)
**Exposure time:** 4 hour(s)
**Value:** > .237 mg/l

**Method:** other: in house protocol
**Year:** 1981
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 4 hour exposure period and subsequent 14 day observation period.

CLINICAL SIGNS: No signs of toxicity. All animals gained

weight normally over the observation period.

NECROPSY FINDINGS: None reported.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Blair 1981
Hayes Consultancy Service Bromley, Kent

**Test substance:** Tradename Dobanol 91 Type B

**Conclusion:** The rat 4 hour inhalational LC50 for Dobanol 91 was found to be >0.237 mg/l (near saturated vapour concentration). There were no signs of toxicity at this exposure level.

This study was reported in Iuclid 2000.

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit, Sittingbourne, Kent, UK
- Age: 11 weeks approx.
- Weight at study initiation: males 327-391g; females 190-240g

- Number of animals: 5M+5F/group
- Controls: none

ADMINISTRATION:
- Type of exposure: 4 hour inhalation exposure, whole body
- Concentrations: Two separate exposures were made as follows firstly to an atmosphere containing 0.212 mg/l of the more volatile components of Dobanol 91 and secondly to an atmosphere containing 0.237 mg/l of the less volatile components (atmospheres were analysed continuously throughout exposure using a total carbon analyser and flame ionisation detector). In both cases the test atmospheres were near saturated.
- Type or preparation of particles: vapour

EXAMINATIONS: Clinical signs were continuously observed for the first 30 minutes of exposure then at 15 minute intervals throughout exposure and twice daily thereafter throughout the 14 day observation period. Initial and terminal bodyweights were recorded. Gross post mortem examination was carried out on all animals.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions, not GLP but subject to QA audit.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (8) (20)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: CD strain rat (remote Sprague-Dawley origin)
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 2000 mg/kg
**Value:** > 2000 mg/kg bw

**Method:** OECD Guide-line 402 "Acute dermal Toxicity"
**Year:** 1987
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure and observation periods.

CLINICAL SIGNS: No clinical signs of intoxication, all animals achieved expected body weight gains.

NECROPSY FINDINGS: No treatment related changes. Fluid distension of the uterus in one female was not considered treatment related as this is a common finding among female CD rats.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.

**Source:** Shell 1996b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (CD)
- Source: Charles River, Margate, Kent, UK
- Age: young adults
- Weight at study initiation: on day of dosing males 213-306, females 204-236.
- Group size: 5M+5F
- Controls: No

ADMINISTRATION: 24 hour dermal occluded
- Area covered: 5cm X 5cm
- Occlusion: gauze patch occluded with aluminium foil held in place with waterproof plaster bandage.
- Vehicle: none
- Doses: 2000 mg/kg
- Removal of test substance: Gentle wiping with wet disposable tissues 24 hours after administration.

EXAMINATIONS: Observations of clinical signs were made several times on day 1 and once daily thereafter. Bodyweights were recorded the day before dosing on the day of dosing and at 8 and 15 days in the observation period. All animals were subject to gross necropsy consisting of internal and external examination. Sections of major anomalies are taken but not examined routinely.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The dermal LD50 (24 hour occluded) for Linevol 79 was found to be >2000 mg/kg in this limit test.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (32)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 8
**Vehicle:** other: undiluted
**Doses:** 2 ml/kg (1600 mg/kg)

**Value:** > 1600 mg/kg bw

**Method:** other: Noakes & Sanderson, 1969
**Year:** 1969
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4
**Result:** MORTALITY: All animals survived the exposure and observation periods

APPLICATION SITE: No irritation reported.

CLINICAL SIGNS: None observed.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.
**Source:** Cassidy & Clark, 1978b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall), Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F
- Controls: No

ADMINISTRATION: 24 hour occluded dermal application
- Area covered: not reported applied to shorn dorsolumbar skin.
- Occlusion: aluminium foil and waterproof plaster.
- Vehicle: undiluted
- Total volume applied: 2 ml/kg
- Doses: 2 ml/kg
- Removal of test substance: washed with tepid dilute detergent solution.

EXAMINATIONS: Mortality and clinical signs during the 9 day observation period.
**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The rat dermal LD50 for Linevol 79 following a 24 hour occluded exposure to rat skin was >1600 mg/kg. No signs of toxicity were observed.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
18-JUL-2005 (12)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: undiluted
**Doses:** 2 ml/kg
**Value:** > 1600 mg/kg bw

**Method:** other: Noakes and Sanderson, 1969
**Year:** 1969
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure and observation periods

APPLICATION SITE: No irritation reported.

CLINICAL SIGNS: None observed.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Source:** Cassidy and Clark 1978
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall), Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 4M+4F
- Controls: No

ADMINISTRATION: 24 hour occluded dermal application
- Area covered: not reported applied to shorn dorsolumbar skin.
- Occlusion: aluminium foil and waterproof plaster.
- Vehicle: undiluted
- Total volume applied: 2 ml/kg
- Doses: 2 ml/kg
- Removal of test substance: washed with tepid dilute detergent solution.

EXAMINATIONS: Mortality and clinical signs during the 9 day observation period.

**Test substance:** Tradename Dobanol 91 C6-12 alcohols Type B

**Conclusion:** The rat dermal LD50 for Dobanol 91 following a 24 hour occluded exposure to rat skin was >1600 mg/kg. No signs of toxicity were observed.

This study was reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (11) (20)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit

**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**PDII:** 2.5
**Result:** irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: individual 24+72 hour scores abraded skin 1, 1.5, 1.5 (group mean 1.35); intact skin 1.75, 1.75, 1.5 (group mean 1.65)
- Oedema: individual 24+72 hour scores abraded skin 0.5, 1, 1.25 (group mean 0.9); intact skin 1, 1, 1.25 (group mean 1.05)

REVERSIBILITY: Erythema and oedema persisted over the 7 day observation period with group mean 7 day values being for abraded skin erythema 1.2 and oedema 0.7 and for intact skin erythema 1.5 and oedema 1.

OTHER EFFECTS: None reported.

PII: 2.5
**Source:** Cassidy & Clark, 1978b
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: male
- Source: Ranc Rabbit, Crawley, Sussex, UK
- Number of animals: 3
- Controls: Not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2X2 cm
- Occlusion: Occluded
- Vehicle: None
- Exposure period: 224 hours
- Postexposure period: 7 days
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours and 7 days.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** Linevol 79 is a skin irritant following 24 hour occluded exposure to rabbit skin according to either EU criteria or the GHS classification system (category 2) based on persistance of the response at the end of the 7 day observation period.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (12)

**Species:** other: New Zealand White rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** other: undiluted
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores are 0.7, 2.3 and 2.7 (group mean 1.9)
- Oedema: Individual 24+48+72 hour scores are 0.7, 1.3 and 1.3 (group mean 1.1)

REVERSIBILITY: All scores for erythema and oedema were 0 at day 10.

OTHER EFFECTS: Erythema extended beyond the test site in 2 animals at 24 hours and in all animals at 48 and 72 hours and remained beyond the test site in one animal at day 7. Fissuring was also observed in this single animal at day 7. Loss of elasticity was noted from 48 hours after removal of dressings until day 10. Exfoliation was observed from day 7 persisting in one animal until day 16 while lack of hair growth was observed in all animals from day 10 until the end of the study on day 16.

**Source:** Rees 1996a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: Outbred New Zealand White
- Sex: Female
- Source: Froxfield Farm, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.25 -2.5 kg
- Number of animals: 3
- Controls: Untreated site on same animals with semi-occlusive dressing.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 3 X 2 cm
- Occlusion: Semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 16 days
- Removal of test substance: with warm water & paper tissues

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours then at days 7, 10, 13 and 16.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** Linevol 79 is considered a skin irritant using both the EC and GHS classification schemes (category 2).

**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (26)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 3
**PDII:** 2
**Result:** irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual mean 24+72 hour scores abraded skin 1.25, 2, 1.25 (group mean 1.5) intact skin 1.25, 2, 1.5 (group mean 1.55)
- Oedema: Mean 24+72 hour score intact and abraded skin 0.5

REVERSIBILITY: Group mean scores at 7 days were erythema intact skin 0.8, abraded skin 0.7; oedema intact skin 1, abraded skin 0.8.

OTHER EFFECTS: None reported. PII is 2.
**Source:** Cassidy & Clark, 1978
**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: Ranch Rabbits, Crawley , Sussex, UK
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Same animals

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2cm X 2cm
- Occlusion: Occlusive
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 24 hours to intact and abraded skin.
- Postexposure period: 7 days
- Removal of test substance: Not reported

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours and 7 days.

**Test substance:** Tradename Dobanol 91 C6-12 alcohols Type B
**Conclusion:** Dobanol 91 is a skin irritant following 24 hour occluded exposure to rabbit skin according to either EU criteria or the GHS classification system (category 2) based on persistance of the response at the end of the 7 day observation period.

This result is reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions

Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (11) (20) (20)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+72 hour scores 3 animals scored 2 the remaining 3 scored 1.7. Group mean 24+48+72 hour score 1.83.
- Oedema: Individual 24+48+72 hour scores 3 animals scored 1.3 the remaining 3 scored 1.7. Group mean 24+48+72 hour score 1.5.

REVERSIBILITY: By day 7 all scores for oedema were 0. There was evidence that erythema was also regressing the group mean 7 day score being 1.

OTHER EFFECTS: None reported.

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Lial 111 C6-12 alcohols Type A
**Conclusion:** Following a 4 hour occluded exposure to rabbit skin, LIAL 111 (C11) was not a skin irritant according to EU criteria (group mean 24+48+48 hour scores <2). With erythema scores all >=1.5 LIAL 111 is classifiable as a mild (slight) skin irritant according to the GHS.

**Reliability:** (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (6)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** irritating
**EC classificat.:** irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hours)
- Cornea: individual scores all 2 (group mean score 2)
- Iris: individual scores all 1 (group mean score 1)
- Conjuntivae (Redness): individual scores all 2 (group mean scores 2)
- Conjunctivae (Chemosis): individual scores 1.3, 1.3, 0.7 (group mean score 1.1)

DESCRIPTION OF LESIONS: Crimson-red conjunctival appearance, very slight/slight chemosis and discharge, iritis and slight corneal opacity covering up to the entire corneal surface were observed during the first 72 hours post instillation. Corneal stippling observed in one animal at 48 hours.

REVERSIBILITY: After 7 days conjunctivial injection was apparent in all animals (grade 1 some vessels definitely injected) persisting in two animals until day 22. By day 29 all eyes were overtly normal.

OTHER EFFECTS: Very slight initial pain response.

**Source:** Rees 1996b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: 5 months
- Weight at study initiation: 2.7 - 2.97 kg
- Number of animals: 3
- Controls: Untreated eye.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 29 days

EXAMINATIONS
- Scoring system: As OECD guideline
- Observation period: 29 days
- Tool used to assess score: ophthalmoscope or pencil beam torch. From 24 hours as required one drop fluorescein used to assess corneal injury.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C

**Conclusion:** Linevol 79 is an eye irritant according to EU criteria based on a mean 24+48+72 hour score for iritis of 1 in all test animals. Based on scores for conjunctivitis and corneal opacity of 2 and iritis of 1 and eventual reversibility of the response by 29 days (effects at 22 days were minimal) Linevol 79 is considered a category 2A eye irritant according to GHS criteria.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (27)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .2 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): group mean score 0.8
- Conjunctivae (Chemosis): 0.27

DESCRIPTION OF LESIONS: Individual scores were not reported.

REVERSIBILITY: All scores at day 7 were 0.

OTHER EFFECTS: Discharge was observed at 48 and 72 hours after instillation.

**Source:** Cassidy & Clark, 1978b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: not reported
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit.
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.2 ml

- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: not reported
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: Not reported

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** Linevol 79 is not an eye irritant according to EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (12)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .2 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** none
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0.9
- Iris: 0
- Conjunctivae (Redness): 2
- Conjunctivae (Chemosis): 1.4

DESCRIPTION OF LESIONS: No individual scores reported. Some conjunctival discharge reported at 24 and 48 hours after instillation.

REVERSIBILITY: All scores 0 by day 7.

OTHER EFFECTS: Slight initial pain response.
**Source:** Cassidy and Clark 1978
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: not reported
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit.
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 3
- Controls: Untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.2 ml
- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: not reported
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: Not reported

**Test substance:** Tradename Dobanol 91 C6-12 alcohols Type B

**Conclusion:** Dobanol 91 is not an eye irritant according to EU criteria. Based on scores for conjunctival redness (group mean 24+48+72 hour score 2) with reversibility within 7 days Dobanol 91 can be considered a category 2B irritant under GHS criteria.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (11) (20)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Exposure Time:** unspecified
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1985
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: individual scores all 0 (group mean score 0)
- Iris: individual scores all 0 (group mean score 0)
- Conjunctivae (Redness): individual scores all 2 (group mean score 2)
- Conjunctivae (Chemosis): individual scores 4 rabbits 1, 2 rabbits 1.3 (group mean score 1.11)

REVERSIBILITY: Conjunctival redness and chemosis persisted to 7 days. Individual scores for redness were 4 rabbits grade 1, 2 rabbits 0 (group mean score 0.66) and for chemosis wer 3 rabbits grade 1, 3 at 0 (group mean score 0.5)

OTHER EFFECTS: None reported

**Source:** Biolab SGS 1985a

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: Unknown
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml

- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: As guideline
- Observation period: 7 days
- Tool used to assess score: direct observation and UV lamp

**Test substance:** Tradename Lial 111 C6-12 alcohols Type A

**Conclusion:** Lial 111 is not considered an eye irritant according to EU criteria, although there was evidence of conjunctival irritation at 7 days this was noticeably less than at 72 hours. Using GHS criteria Lial 111 is a category 2A irritant based on 24+48+72 hour scores for conjunctival redness of 2 in all rabbits and persistence to 7 days.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions. Observation period could have been extended to fully observe reversal of effects.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (5)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction 50 % intracutaneous
**2nd:** Induction 50 % occlusive epicutaneous
**3rd:** Challenge 5 % occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: propylene glycol
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** OECD Guide-line 406 "Skin Sensitization"
**Year:** 1996
**GLP:** yes

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: Intradermal administration resulted in slight erythema which had regressed by day 7. Some animals developed eschar by day 7 and pallor, skin discoloration was also reported. There was no obvious dose relationship although concentrations from 1 to 50% were tested. Following topical induction eschar was obsered at sites receiving undiluted Linevol 79, concentrations of 10 -30% resulted in exfoliation only, erythema was not observed. The topical challenge resulted only in discoloration in one animal and exfoliation in several.

RESULTS OF TEST
- Sensitization reaction: Challenge application of 30% v/v linevol 79 in propylene glycol gave rise to eschar in 9 test and 3 control animals. A further 10 test and 5 controls showed slight erythema. Exfoliation was present in 2 test animals.

Challenge application of 5% Linevol 79 resulted in eschar formation in 1 test animal and slight erythema in 1 test animal, exfoliation was observed in 3 test animals.

No dermal reaction was evident following challenge application of propylene glycol alone.

Irritation in the main test was obviously more marked than in the pilot study. While there was a slight increase in the incidence of significant responses in the test group this was attributed to primary irritation. Total significant responses in the test group were 19/20 for the 30% challenge and 8/10 for controls. Following challenge with 5% Linevol 79 in propylene glycol 2/20 test and 0/10 controls showed a significant response. A response in 30% of test animals is considered positive.

**Source:** Rees 1996c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: Dunkin Hartley
- Sex: male and female
- Source: David Hall, Darley Oaks, Staffordshire UK
- Age: 6-8 weeks
- Number of animals: Test group 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: adjuvant
- Preparation of test substance for induction: and 50% in propylene glycol with Freunds Complete Adjuvant (FCA).
- Preparation of test substance for induction: In propylene glycol
- Induction schedule: Primary induction intradermal day 1, 2nd induction topical day 8.
- Concentrations used for induction: 50% in propylene glycol.
- Concentration in Freuds Complete Adjuvant (FCA): 50%
- Challenge schedule: Day 22
- Concentrations used for challenge: 30% and 5%
- Rechallenge: No
- Positive control: Not reported

EXAMINATIONS
- Grading system: Magnusson & Kligman
- Pilot study: Yes

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C

**Conclusion:** Linevol 79 was not a skin sensitiser in the guinea pig maximisation test. A slight increase in significant reactions in the test group was attributed to primary irritation.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

18-JUL-2005 (28)

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction .1 % intracutaneous
**2nd:** Induction 100 % occlusive epicutaneous
**3rd:** Challenge 50 % occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: corn oil
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: M&K guinea pig maximization test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: No details given.

RESULTS OF TEST
- Sensitization reaction: 0/20 treated and 0/10 controls at 24 and 48 hours. Result negative.
- Clinical signs: None in test or controls.
- Rechallenge: Not carried out.

**Source:** Cassidy & Clark, 1978b
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: P-strain
- Sex: male & female
- Source: Shell Toxicology Lab (Tunstall) breeding unit.
- Age/weight: Not reported
- Number of animals: 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: Maximization (M&K)
- Preparation of test substance for induction: In corn oil
- Preparation of test substance for challenge: In corn oil
- Induction schedule: Intradermal injection followed one week later by topical application (48 hour occlusive).
- Concentrations used for induction: 0.1% intradermal, 100% topical (48 hour occlusive).
- Concentration in Freuds Complete Adjuvant (FCA): not reprted
- Challenge schedule: 2 weeks after topical induction, 24 hour topical challenge.
- Concentrations used for challenge: 50% in corn oil.
- Rechallenge: No
- Positive control: Not reported

EXAMINATIONS
- Grading system: 4 point scale -ve, trace, +ve, ++ve
- Pilot study: Initial irritation screen, no details given.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** Dobanol 79 was not a skin sensitiser in guinea pigs when tested using the M&K maximisation procedure.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
05-DEC-2005 (12)

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction .1 % intracutaneous
**2nd:** Induction 10 % occlusive epicutaneous
**3rd:** Challenge 5 % occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: corn oil
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: M&K guinea pig maximization test
**Year:** 1978

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: No details given.

RESULTS OF TEST
- Sensitization reaction: 0/20 treated, 0/10 controls at 24 and 48 hours, result negative.
- Clinical signs: None in test or controls.
- Rechallenge: Not carried out.

**Source:** Cassidy and Clark 1978
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: P-strain
- Sex: male & female
- Source: Shell Toxicology Lab (Tunstall) breeding unit.
- Age/weight: Not reported
- Number of animals: 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: Maximization (M&K)
- Preparation of test substance for induction: In corn oil
- Preparation of test substance for challenge: In corn oil
- Induction schedule: Intradermal injection followed one week later by topical application (48 hour occlusive).
- Concentrations used for induction: 0.1% intradermal, 10% topical.
- Concentration in Freuds Complete Adjuvant (FCA): 50:50
- Challenge schedule: 2 weeks after topical induction, 24 hour topical challenge.
- Concentrations used for challenge: 5% in corn oil.
- Rechallenge: No
- Positive control: Not rpeorted

EXAMINATIONS
- Grading system: 4 point scale -ve, trace, +ve, ++ve
- Pilot study: Initial irritation screen, no details given.

**Test substance:** Tradename Dobanol 91 C6-12 alcohols Type B
**Conclusion:** Dobanol 91 was not a skin sensitiser in guinea pigs when tested using the M&K maximisation procedure.

This result was reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
05-DEC-2005 (11) (20)

## 5.4 Repeated Dose Toxicity

**Type:** Sub-acute
**Species:** rat **Sex:** male/female
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 7 days
**Frequency of treatment:** Daily for 7 consecutive days
**Post exposure period:** none
**Doses:** 5 ml/kg/day = 4175 mg/kg bw
**Control Group:** yes

**NOAEL:** < 4175 mg/kg bw
**LOAEL:** = 4175 mg/kg bw

**Method:** other
**Year:** 1970
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were no deaths. Irritability and diarrhoea were the only clinical signs of intoxication. Histological examination revealed hyper and parakeratosis of the cardiac stomach and periportal cytoplasmic vacuolation in the liver of some of the treated rats. Focal inflammation of the submucosa was not uncommon. There were no other treatment related histopathological changes.
**Source:** Brown et al. 1970.

Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Weight at study initiation: 150-250 g
- Number of animals: 8M+8F test group, 20M+20F controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 7 days
- Type of exposure: oral gavage
- Post exposure period: Carworth Farm E
- Vehicle: none
- Total volume applied: 5 ml/kg
- Doses: single dose 5 ml/kg (4175 mg/kg/day)

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: daily
- Mortality: daily
- Body weight: not reported
- Haematology, Biochemistry, Urinalysis: not carried out

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: full autopsy
- Microscopic: major viscera

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** Screening study which confirms the irritative effect of lower chain alcohols on the digestive tract.
**Reliability:** (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment. Screening study only.
18-JUL-2005 (10) (20)

**Type:** Sub-acute
**Species:** rat **Sex:** male
**Strain:** Wistar
**Route of administration:** gavage
**Exposure period:** 14 days
**Frequency of treatment:** daily
**Post exposure period:** no
**Doses:** 1 mmol/kg/day (128 mg/kg/da7)
**Control Group:** yes, concurrent vehicle

**Method:** other
**Year:** 1984
**GLP:** no data

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** In vivo studies: There were no effects on relative testes weight, relative liver weight showed a slight* significant increase with 3,5,7-trimethyl hexanol. The postive control DEHP showed a clearly significant increase** in relative liver weight. There were no significant changes in testes weight relative to controls. Histopathological examination of the liver revealed no treatment related changes. Only the positive control DEHP showed any peroxisome proliferation or effects on cholesterol or triglycerides catalase was unaffected by treatment.
In vitro levels of palmitoyl CoA oxidase were increased only in the positive control group (MEHP).

**Source:** Rhodes et al, 1984
Hayes Consultancy Service Bromley, Kent

**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce hepatomegaly, peroxisome proliferation or hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any indication of testicular atrophy.

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol 300 as a vehicle and the test compounds a common dose level (on a molar basis) of 1 mmol/kg/day for 14 days. At the end of this period liver and testes weights were recorded. The liver was removed and samples taken for light and electron microscopy. The remaining liver was homogenised and prepared for assay of total catalase and CN-insensitive palmitoyl CoA oxidation. In vitro hepatocyte cultures were also prepared and the same compounds assessed for effects on CN-insensitive palmitoyl CoA oxidase activity after 72 hours incubation.

Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C

**Conclusion:** None of the alkanols investigated at dose levels of 1 mMol/kg showed any evidence of peroxisome proliferation, hepatomegaly, hepatomegaly, or hypolipidaemia. Testes weights were also unaffected by treatment.

**Reliability:** (2) valid with restrictions
Research publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

18-JUL-2005 (30)

**Type:** Sub-acute
**Species:** rat **Sex:** male/female
**Strain:** other: Carworth Farm E
**Route of administration:** gavage
**Exposure period:** 7 days
**Frequency of treatment:** daily
**Post exposure period:** none
**Doses:** 5ml/kg (4150 mg/kg/day)
**Control Group:** yes, concurrent vehicle
**NOAEL:** < 4150 mg/kg bw
**LOAEL:** = 4150 mg/kg bw

**Method:** other: see text
**Year:** 1970
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** There were no deaths. Irritability and diarrhoea were the only clinical signs of intoxication. Histological examination revealed hyper and parakeratosis of the cardiac stomach and periportal cytoplasmic vacuolation in the liver of some of the treated rats. Focal inflammation of the submucosa was not uncommon. There were no other treatment related histopathological changes.
**Source:** Brown et al, 1970
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS
- Weight at study initiation: 150-250 g
- Number of animals: 8M+8F test group, 20M+20F controls

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 7 days
- Type of exposure: gavage
- Post exposure period: none
- Vehicle: none
- Total volume applied: 5 ml/kg
- Doses: 5 ml/kg (4150 mg/kg)

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Not reported

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full necropsy
- Microscopic: Major viscera

**Test substance:** Tradename Linevol 911 C6-12 alcohols Type B
**Conclusion:** Screening study which confirms the irritative effect of lower chain alcohols on the digestive tract.

Reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Study reasonably well documented, meets generally accepted scientific principles, acceptable for assessment. Screening test.
18-JUL-2005 (10) (20)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames test)
**System of testing:** Salmonella typhimurium strains TA98, TA100, TA 1535, TA 1538
**Concentration:** 50, 158, 500, 1590 and 5000 ug/plate
**Cytotoxic Concentration:** no cytotoxicity observed at any concentration.
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: similar to OECD 471
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: no increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Precipitation not reported.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No cytoxicity observed at the highest test concentration of 5000 ug/plate.

**Source:** Shell 1996.
Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA1535, 1538, 98 and 100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 50, 158, 5000 , 1580 and 5000 ug/plate
- Number of replicates: triplicate
- Application: Pour plate, vehicle DMSO
- Positive and negative control groups and treatment: Negative controls, solvent (DMSO) and untreated bacteria. Postive controls sodium azide 2 ug/plate, 2-aminoanthracene 2 ug/plate, 9-aminoacridine 80 ug/plate, 2-nitrofluorene 1 ug/plate, benzo[a]pyrene 5 ug/plate
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Not mentioned in the report assume as OECD 471.

**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The C6-12 alcohol Linevol 79 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 5000 ug/plate. All positive controls gave an appropriate response.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
18-JUL-2005 (34)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** In common with other members of the aliphatic alcohols category C6-12 alcohols (Types A,B,C and D) contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the range of category members (linear and essentially linear), including a negative Ames test for C6-12 alcohols type C, are negative. Results from in vivo studies with other category members and/or supporting substances provide evidence that these alcohols are not genotoxic in vivo.

Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** As prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline studies or publications with sufficient detail for assessment.

25-OCT-2005 (36) (38) (43)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

-

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C6-12 alcohols (both linear and essentially linear) are not expected to be developmental toxicants in the absence of maternal toxicity.

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for developmental toxicity are based are either comparable to guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (36) (37) (43)

## 5.8.3 Toxicity to Reproduction, Other Studies

**Type:** other: comparative study including measurement of testes weight
**In Vitro/in vivo:** In vivo
**Species:** rat
**Strain:** Wistar **Sex:** male
**Route of administration:** gavage
**Exposure period:** 14 days
**Frequency of treatment:** daily
**Duration of test:** 14 days
**Doses:** 1 mmol/kg/day (128 mg/kg/day)
**Control Group:** yes, concurrent vehicle

**Method:** other: see text
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Following repeated oral administration of equimolar dose levels of various alkanols to male rats for a period of 14 days there were no statistically significant differences in body weight gain, or relative liver or testes weights.
**Source:** Rhodes, 1984
**Test condition:** This study was carried out to determine whether various alkanols in the C6-13 range produce similar effects to those observed with diethyl hexyl phthalate (DEHP) and its metabolite 2-ethyl hexanol in terms of hepatomegaly, peroxisome proliferation, hypotriglyceridaemia. As part of the study testes weights were recorded to see if there was any indication of testicular atrophy (a known effect of DEHP).

The test materials were administered to groups of male Wistar rats (10/control group, 5/treated group) by gavage using polyethylene glycol as a vehicle at a common dose level (on a molar basis) of 1 mmol/kg/day for 14 days. At the end of this period testes weights were recorded together with various indices of liver toxicity (see chapter 5.4 Repeated dose toxicity for further details).

Actual dose levels on a mg/kg/day basis were as follows:

2-ethyl hexanol 130 mg/kg/day
Iso-octanol 130 mg/kg/day
3,5,7-trimethylhexanol 144 mg/kg/day
Iso-nonanol 144 mg/kg/day
Iso-decanol 168 mg/kg/day
Tridecanol 184 mg/kg/day

Mixed branched & straight chain
Alphanol C7-9 128 mg/kg/day
Synprol C13-15 209 mg/kg/day

Straight chain
Alfol C6-10 (Alfol 610) 133 mg/kg/day
Linevol C7-9 (Linevol 79) 128 mg/kg/day
**Test substance:** Tradename Linevol 79, C6-12 alcohols Type C
**Conclusion:** The results of this study provide supportive evidence for a

lack of effect of a range of alcohols on the testes following repeated oral administration as evidenced by lack of effect on relative testes weights.

**Reliability:** (2) valid with restrictions
Research publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

19-JUL-2005 (30)

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 68855-56-1
**CAS No.** 68855-56-1
**EINECS Name** Alcohols, C12-16
**EC No.** 272-490-6
**TSCA Name** Alcohols, C12-16

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 11-MAY-2006
**Revision date:**
**Date of last Update:** **11-MAY-2006**

**Number of Pages:** **76**

**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

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08-MAR-2006

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23-AUG-2005

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**Remark:** Consortium Member
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**Remark:** Consortium Member
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**Remark:** Consortium Member
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**Remark:** Consortium Member
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**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |

| | |
|---|---|
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential.
Non-confidential data are summarised here.
Of the commercial products associated with the Consortium members, those identified as C12-16 alcohols, CAS 68855-56-1 are 40-100% linear.

The substance comprises C12-16 alcohols. Components of even or even and odd chain length, in the range C8-C18 are present.

Commercial products marketed under this CAS number fall into three types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A, Type B and Type C.

Type A products are >40% linear. The substance comprises >95% C12, 13, 14 and 15. Components of even and odd chain length, in the range C10-C17 are present.

Type B products are 100% linear. The substance comprises >80% C12 and 14, <20% C16. Components of even chain length, in the range C8-C18 are present.

Type C products are 100% linear. The substance comprises <10% C12, >90% C14 and 16. Components of even chain length, in the range C10-C18 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C12-16 (CA INDEX NAME)
Alfol 1216
Alfol C
C12-16 alcohols
C12-16-alcs.

CO 1214
Conol 20F
Conol 20HM
Kalcohl 2470
Kalcohl 4250
Lial 145
Lorol 1214
Lorol 1214A

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C12-16 alcohols.

Composition is described in section 1.1.1, General Substance Information

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.
Commercial production figures for specific CAS, or narrow

ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >5 - 250 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >10 000 - 500 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (4) (31) (43)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 35 Lubricants and additives
**Extra details on use category:** No extra details necessary
No extra details necessary

**Emission scenario document:** not available

19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Paints Lacquers and Varnishes
19-SEP-2005

**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification NWG or 1 ID No. 1482 and 656
05-AUG-2005 (45)

## 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

## 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

## 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-16 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed

up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

11-AUG-2003

## 2.1 Melting Point

**Value:** = 21 degree C
**Decomposition:** no at degree C
**Sublimation:** no

**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number
21-OCT-2005

**Remark:** Solidification point: 18 - 22 degr. C
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
21-OCT-2005 (34)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
21-OCT-2005

## 2.2 Boiling Point

**Value:** = 255 - 310 degree C at 1013 hPa

**Method:** other: DIN 51751

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
21-OCT-2005 (34)

**Value:** = 265 - 295 degree C at 1013 hPa
**Decomposition:** no

**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
21-OCT-2005

**Value:**

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Type:** density
**Value:** = .831 g/cm³ at 20 degree C

**GLP:** no data

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
**Flag:** Critical study for SIDS endpoint
21-OCT-2005

**Type:** density
**Value:** = .82 - .83 g/cm³ at 30 degree C

**Method:** other: DIN 51757 Verf. B

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
21-OCT-2005 (34)

**Value:** = .83 at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** It is not possible to determine which compositional Type was

tested.
**Reliability:** (4) not assignable
11-OCT-2005 (28)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No reliable measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
21-OCT-2005 (40)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00025 - .0016 hPa at 25 degree C

**Method:** other (calculated): by composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.00054 value hPa
Type B: 0.0016 value hPa
Type C: 0.00025 value hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 6

**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (4) not assignable
This information was obtained from secondary literature (company product data) and cannot be validated further.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (37)

**Partition Coeff.:** octanol-water
**log Pow:** = 5.4 - 6.7 at 25 degree C

**Method:** other (calculated): based on values of components, and amended SRC KOWWIN v1.66
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The substance has a range of components, as described in section 1.1-1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Result:** Type A and B: 5.4 - 6.7
Type C: 5.4 - 6.4
**Reliability:** (2) valid with restrictions
The value was predicted using reliable measured values of components, and an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .8 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (11) (28)

**Solubility in:** Water
**Value:** = .42 - 3.2 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.69 mg/l at a loading rate of 1000 mg/l
Type B: 3.2 mg/l at a loading rate of 1000 mg/l
Type C: 0.42 mg/l at a loading rate of 1000 mg/l
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** = .8 mg/l at 20 degree C

**Method:** other
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Shell Chemicals UK Ltd Chester
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
11-OCT-2005 (35)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 132 degree C
**Type:** closed cup

**Method:** other
**GLP:** no

**Remark:** Figure quoted is typical
**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from company product data reported in the public IUCLID 2000 CD-ROM, and cannot be validated further. Insufficient test substance compositional

data were reported for the test results to be reliably assigned to the CAS number.
21-OCT-2005 (17)

**Value:** ca. 140 degree C
**Type:** closed cup

**Method:** other: DIN 51758
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from company product data reported in the public IUCLID 2000 CD-ROM, and cannot be validated further. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005 (34)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of flashpoint. It is not possible to estimate with confidence what the flashpoint might be.
21-OCT-2005

## 2.8 Auto Flammability
-

## 2.9 Flammability
-

## 2.10 Explosive Properties
-

## 2.11 Oxidizing Properties
-

## 2.12 Dissociation Constant
-

## 2.13 Viscosity
-

## 2.14 Additional Remarks
-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.

**Flag:** Critical study for SIDS endpoint

18-JAN-2006 (3)

**Type:** air
**Light source:** Sun light
**Rel. intensity:** = 100 based on Intensity of Sunlight
**Conc. of subst.:** at 15 degree C
**INDIRECT PHOTOLYSIS**
**Sensitizer:** OH
**Conc. of sens.:** 1000000 molecule/cm³
**Rate constant:** = .00000000001358 cm³/(molecule * sec)
**Degradation:** = 50 % after 19.2 hour(s)

**Method:** OECD Guide-line draft "Photochemical Oxidative Degradation in the Atmosphere"
**Year:** 1990
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Shell Chemicals UK Ltd Chester
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. Further review of the original source, to reassess the reliability, would not alter the overall conclusions concerning this end point. A source of higher reliability is available.

**Flag:** Critical study for SIDS endpoint

18-JAN-2006 (27)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and

would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
07-JAN-2005

### 3.1.3 Stability in Soil

-

### 3.2.1 Monitoring Data (Environment)

-

### 3.2.2 Field Studies

-

### 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** Type A:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 177000 |
| TGD Non-hydrophobics method: | Koc = 6400 - 23100 |
| TGD Alcohols method: | Koc = 390 - 1020 |
| SRC PCKOCWIN method: | Koc = 330 - 2050 |

Type B:
TGD Hydrophobics method: Koc = 27600 - 307000
TGD Non-hydrophobics method: Koc = 6400 - 30100
TGD Alcohols method: Koc = 390 - 1240
SRC PCKOCWIN method: Koc = 330 - 3790

Type C:
TGD Hydrophobics method: Koc = 27600 - 307000
TGD Non-hydrophobics method: Koc = 6400 - 30100
TGD Alcohols method: Koc = 390 - 1240
SRC PCKOCWIN method: Koc = 330 - 3790

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 10 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 29 day(s)
**Degradation:** = 59 % after 28 day(s)
**Result:** other: not readily biodegradable
**Kinetic:** 3 day(s) = 10 %
6 day(s) = 33 %
15 day(s) = 49 %
29 day(s) = 61 %
**Control Subst.:** other: Sodium benzoate

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A five-day bacterial inhibition test was performed under the conditions of the Closed Bottle Test. In a subsequent Modified Sturm Test, the test material was added to two vessels containing mineral salts medium and activated sludge to give a nominal test concentration of 10 mgC/l. Control vessels comprised two containing inoculated mineral salts medium alone and one containing inoculated mineral salts plus sodium benzoate (10 mgC/l). Test and control vessels were aerated for 29 days with air that had been treated to remove CO2.
**Remark:** The following validity criteria were met (1) the reference substance reached the pass level within 14 days,
(2) Parallel assays did not differ by more than 20%, (3) Cumulative CO2 production in the controls after 29 days (77.8 and 80.1 mgCO2) was within the acceptable range for this assay system (recommended maximum = 120 mgCO2 for a three litre culture).

**Result:** Kinetic of control substance: 3 days = 39%
6 days = 68%
15 days = 82%
28 days = 87%
The substance attained < 60% degradation in 28 days, therefore it cannot be considered readily biodegradable, although significant degradation was observed.
Mean cumulative CO2 production by the mixtures containing the test substance at 10 mgC/L was equivalent to 10% of the theoretical value after three days and 61% after 29 days. A degradation plateau was not achieved in this test. The substance degraded 45% in the 10 day window. The material cannot be considered readily biodegradable but is inherently biodegradable. The reference substance, Sodium benzoate degraded by 89% after 29 days.
**Test condition:** Concentration of inoculum: 30 mg solids/l
Test volume: not reported
Temperature: 21.2 - 23.9 C
pH: 7.4 - 7.6
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
Guideline study, not conducted to GLP.
**Flag:** Critical study for SIDS endpoint
05-OCT-2005 (22)

**Type:** aerobic
**Inoculum:** other: settled sewage - origin unknown
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 83 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:** 11 day(s) = 64 %
15 day(s) = 70 %
21 day(s) = 77 %
26 day(s) = 82 %
28 day(s) = 83 %

**Method:** other: Sturm-Weaver test procedure
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** A modification of the Sturm Weaver test was performed. 6% CaCl2 on DOBS PT active matter is added to stabilise the emulsion. Carbon dioxide free air is passed through the solution. The carbon dioxide evolved during biodegradation is carried to barium hydroxide absorbers by the air stream. Comparing the titration with hydrochloric acid to a phenolphthalein endpoint for the product against that for the blank allows the mass of carbon dioxide evolved to be calculated. The test is continued until plateau conditions are obtained, normally 26-30 days. This method corresponds to OECD 301B, except that the inoculum was taken from an acclimated culture.
**Remark:** It is not stated in the report whether the validity criteria are met.
**Result:** The substance degraded >60% in the 10 day window.
**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (3) invalid
Study was considered invalid due to significant methodological deficiencies, inoculum was acclimated before use.
28-SEP-2005 (42)

**Result:** readily biodegradable

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4.

All components present in compositional Type A are predicted to be readily biodegradable, meeting the ten-day window.

All components present in compositional Types B and C are predicted to be readily biodegradable, though it is uncertain whether the ten-day window would be met or not.

These conclusions are drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.
**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (18)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other
**Year:** 1974
**GLP:** no data
**Year:**
**Method:** The tests were conducted in accordance with the 'Standard Dilution Method' at 20 C for a period of 5 days. This method is described in APHA 'Standard Methods' Nr.219 and was formerly included in the ASTM Standards under Nr. D2329-68. For practical reasons the official Netherlands method NEN 3255 5.4 was used. The only difference in the NEN procedure compared with the others is that consumption of oxygen as a result of nitrification is prevented by the addition of allylthiourea. The test solutions were seeded with 10 ml/l of the effluent of a biological sanitary waste treatment plant.
**Remark:** BOD measurements were expressed as weight of oxygen per weight of chemical (g/g) and, if composition of the product

was known, as a percentage of the theoretical oxygen demand, ThOD (%).
**Result:** Test was also carried out with an adapted seed.
BOD 5 = 1.50 - 1.95 g/g
BOD 5 = 2.26 - 2.41 g/g (adapted)
%ThOD = 62 - 77%(adapted)
>50% degradation, therefore was grouped into good degradability class
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
15-SEP-2005 (12)

**Method:**

**C O D**

**Method:** other
**Year:** 1974
**GLP:** no data
**COD:** = 2.81 mg/g substance
**Method:** In the COD test (ASTM D 1252-67) the oxidizable material present in waste water is oxidised by a standard potassium dichromate solution in 50% sulfuric acid. The mixture is refluxed at about 145 C for two hours. The excess dichromate is then titrated and the COD calculated.
**Result:** The COD was found to be 2.81 g/g.
90% oxidation to water and carbon dioxide was also calculated.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
15-SEP-2005 (13)

**Method:**
**Method:** other: Assessed using methods based on OECD Guideline 301D
**Year:**
**GLP:** no data
**Method:** Triplicate mixtures containing the test substance at nominal concentrations of 5 mg/L and 2.5 mg/L in mineral salts medium inoculated with final effluent were incubated for five days. The COD of the test material was determined by oxidation with an acid-dichromate mixture using a semi-micro procedure.
**Result:** The mean BOD was 0.80 gO2/g. The mean COD was 2.30 gO2/g. The BOD:COD ratio ranged from 31 to 38%. The mean 5 day BOD of Kalcohl 2475 was 35% of its COD.
**Test condition:** Concentration of inoculum: 5 ml/l
Test volume: not reported
Temperature: 20.6-21.2 C
pH: 7.0-7.7
**Test substance:** This result was measured for a commercial product of compositional Type B.
**Reliability:** (2) valid with restrictions
11-OCT-2005 (23)

## 3.7 Bioaccumulation

**BCF:** = 4500 - 45300

**Method:** other: calculated (based on values of components)
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates

**Result:** Type A: BCF estimated as 4500 - 42600
Types B and C: BCF estimated as 7200 - 45300

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** semistatic
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = 100
**LL50 :** = 100 - 300
**Limit Test:** no

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The solubility of the lowest carbon chain length, C12, is 3 mg/l, therefore the LL50 is not reached at the solubility limit.
The test media were produced using a water accommodated fraction (WAF) methodology and sealed vessels since the material was to be tested at loading rates which exceeded the solubilities of some of the components of the mixture

**Result:** RESULTS: EXPOSED
NOEL = 100 mg/l
LL50 = 100-300 mg/l
Based on loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 1
Nature of adverse effects: Died at 48 h

**Source:** Eadsforth et al. 2000.

**Test condition:** TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Brow Well Fisheries Ltd., Hebden, Yorkshire, UK
Weight: 0.99 g
Feeding: Mainstream Trout Diet
Pretreatment: Fish acclimated for at least 12 days prior to start of test
Feeding during test: none
Control group: 1 control group containing 7 fish placed in mains borehole water
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: None
Concentration of vehicle/solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS: Determined to be stable
DILUTION WATER
Source: Laboratory mains tap water (borehole water supplied by 500 ft deep Stanlow well)
Aeration: Not reported
Alkalinity: Not reported
Hardness: 157-181 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Loading rates: 10, 30, 100, 300, and 1000 mg/l
Renewal of test solution: daily
Exposure vessel type: 17 l glass bottles

Number of replicates: 1
Fish per replicate: 7
Test temperature: 14.4-15.2 C
Dissolved oxygen: 6.0-9.6 mg/l
pH mean: 7.7-8.4
Adjustment of pH: none
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: mortality
SAMPLING: Fish observed for toxic symptoms at 3, 24, 48, 72 and 96h
MONITORING OF TEST SUBSTANCE CONCENTRATION: Every 24 hours. The concentration of Neodol 25E in test media reduced by 23-82% over the course of the 72 hour test period.

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (16)

**Type:** static
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 10
**LC50:** = 57
**Limit Test:** no

**Method:** other
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The solubility of the lowest carbon chain length in the compound, C12, is 3 mg/l, therefore the LC50 was not achieved at the solubility limit.

The absence of any measurements of dissolved concentration, at nominal loadings very much greater than the water solubility, suggests the possibility of an artefactual dose-response.

**Result:** RESULTS: EXPOSED
NOEC 10 mg/l
LC50 57 mg/l
Based on nominal concentrations
Sublethal, treatment-related effects were noted at 32 and 100 mg/L and included hyperventilation, darkened pigmentation, and lethargy. At 100 mg/L, all fish appeared normal at 15 minutes but were dead at 24 hours; at 32 mg/L, effects were exhibited from 24 hours onward.
RESULTS: CONTROL
Number/% showing adverse effects: none

**Source:** Huntingdon Life Sciences Ltd. 1996i.

**Test condition:** TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Fish Network Ltd, Devon, UK
Weight: 1.0 g
Feeding: Not reported
Pretreatment: Fish maintained in treated tap water for 14 day period prior to the test
Feeding during test: Not reported

Control group: 1 control group placed in dilution water and 1 group in dilution water containing HCO-40 at the same level as in the test medium at the highest concentration
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: 10 and 1000 mg/l prepared by adding test material mixed with an equal amount of HCO-40 to dilution water
Vehicle, solvent: HCO-40 added to aid dispersion
Concentration of vehicle/solvent: Not reported
Purity/supplier: Huntingdon Life Sciences Ltd.
STABILITY OF TEST CHEMICAL SOLUTIONS
no analysis of control and test media were undertaken
DILUTION WATER
Source: Treated tap water
Aeration: Gentle aeration during test
Alkalinity: not reported
Hardness: 230-254 mg/l CaCO3
Conductance: not reported
TEST SYSTEM
Concentrations: 0.1, 0.32, 1, 3.2, 10, 32, and 100 mg/l
Exposure vessel type: not reported
Number of replicates: 1
Fish per replicate: 5
Test temperature: 13.3-14.7 C
Dissolved oxygen: 75-100%
pH mean: 7.7-8.4
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: mortality
SAMPLING: Not reported
MONITORING OF TEST SUBSTANCE CONCENTRATION: none

**Test substance:** This result was measured for a commercial product of compositional Type B.

**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score are available

19-OCT-2005 (24)

**Type:** static
**Species:** Carassius auratus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = .8
**LC50:** > .8
**Limit Test:** no

**Method:** other: ASTM Method D 1345. Test for Evaluating Acute Toxicity of Industrial Waste Water to Fresh-Water Fishes.
**Year:** 1973
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The experiments were performed in all glass aquaria with 25 L of test solution and 6 or 10 goldfish.
**Result:** The substance was found to be nontoxic at the saturated aqueous solution of 0.8 mg/l.
**Source:** Bridie et al. 1973.
**Test substance:** This result was measured for a commercial product of

compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score, more detail and also indicating no effect at limit of solubility are available
11-OCT-2005 (11)

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 43
**Limit Test:** no

**Method:** other
**Year:** 1977
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The study used fingerlings weighing between 1 and 2 g. Dobanol 25 was dissolved and dispensed into aquaria containing tap water to give logarithmically-spaced concentrations. Each aquarium had 5 fish. The pH was 8.3-8.6.
At all concentrations tested, the water presented the appearance of an opaque solution-dispersion with a thin film on the surface, indicating that the tanks contained amounts of DOBANOL-25 beyond the limit of aqueous solubility. However, a dose response was still observed.
The solubility of C12, the least soluble component of the test substance is 3 mg/l, therefore the LC50 was not achieved at the solubility limit.
**Source:** Shell Toxicology Laboratory 1977.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score, more detailed information and also indicating no effect at limit of solubility are available
11-OCT-2005 (36)

**Type:** other
**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = .54 - 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 2.3 mg/l
Type B: 0.54 mg/l
Type C: >100 mg/l (i.e. predicted to be non-toxic at limit of solubility)
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
30-DEC-2005 (2)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .21 - 2.2 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.2117 mg/l
Type B: 0.25 mg/l
Type C: 2.2 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** < 1

**Limit Test:** yes

**Method:** OECD Guide-line 202
**Year:** 2001
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The test media were produced using a water accommodated fraction (WAF) methodology since the material was to be tested at loading rates which exceeded the solubility of some of the components of the mixture.
After settling (approximately 1 hour) a portion of each WAF and the control were filtered using a 47mm 0.2 um PTFE membrane filter. 1100 ml was initially passed through the filter and discarded before the subsequent 800 ml was collected for use in the tests.
**Remark:** The total measured concentration of the water accommodated fraction of Neodol 25 in test media was 0.27 - 0.36 and 0.20 mg/l at 0 and 24 hours respectively. The mean decrease in levels of the components during the two 24 h periods of use was 38%.
**Result:** RESULTS: EXPOSED
EL50 = <1 mg/l
Based on nominal loading rates
EL50 = <0.2 mg/l
Based on measured loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 1
**Source:** Palmer and Sherren 2001a.
**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Unilever Research, Port Sunlight Laboratory
Age: <24 hours old
Feeding: Algae Chlorella vulgaris
Pretreatment: None
Feeding during test: Not reported
Control group: 2 control groups containing reconstituted fresh water only
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accomadated fractions
Vehicle, solvent: None
STABILITY OF THE TEST CHEMICAL SOLUTIONS:
Considered stable
DILUTION WATER
Source: Reconstituted fresh water
Aeration: Not reported
Alkalinity: Not reported
Hardness: 158 mg/l CaCO3
Conductance: Not reported
TEST SYSTEM
Loading rates: 1 mg/l (loading rate)
Renewal of test solution: Daily
Exposure vessel type: 150 ml Erlenmeyer flasks
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20.2-20.3 C
Dissolved oxygen: 8.0-8.4 mg/l
pH mean: 8.5-8.7
Adjustment of pH: Not reported
Intensity of irradiation: Not reported

Photoperiod: Not reported
TEST PARAMETER: Immobilisation
MONITORING OF TEST SUBSTANCE CONCENTRATION: Every 24 hours. The mean decrease in levels of the components during the two 24 h periods of use was 38%.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (33)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** = 4.6 - 10
**Limit Test:** no

**Method:** other: Based on OECD Guideline 202
**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test media were produced using a water accommodated fraction (WAF) methodology since the material was to be tested at loading rates which exceeded the solubility of some of the components of the mixture.
The reported value, EL50, is the loading rate resulting in 50% immobilisation.
HPLC with florescence detection was used to monitor the concentrations of test solutions.
The solubility of the lowest carbon chain length in the compound, C12, is 0.24 mg/l, therefore the EL50 was greater than the solubility limit.
**Source:** Eadsforth et al. 2000
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
Not key study: Other studies with same reliability score and showing greater toxicity are available.
11-OCT-2005 (16)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** =
**EC50:** = 4.4
**Limit Test:** no

**Method:** other
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This older study was generated by dilution of stock solutions instead of preparing separate WAFs, and using solvent to aid measuring of small quantities of the test substance. The solvent concentration was 5 mg/L. The

concentrations causing effects were greater than the limit of solubility of the least soluble component.
**Source:** Stephenson 1982b.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with a higher reliability score are available
11-OCT-2005 (41)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = .003
**ErL50 :** = .1 - .3
**EbL50 :** = .03 - .1
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of two commercial products to R. subcapitata was determined in sealed 72 h growth inhibition toxicity tests. Algal inocula were exposed to test solutions which were not renewed during the test. The tests were repeated three times for each of the two test items. The test material was directly added to the WAF preparation vessels using ethanol as a carrier (0.1 mL/L). The vessels were then stirred at approximately 100 rpm for a period of approximately 24 hours, before running off the WAFs for use as the test media.
**Result:** RESULTS: EXPOSED
NEODOL 25E
EbL50 = 0.03 - 0.1 mg/l (Area under growth curve)
ErL50 = 0.1 - 0.3 mg/l (Average specific growth rate)
LIAL 125
EbL50 = 0.03 - 0.1 mg/l (Area under growth curve)
ErL50 = 0.1 - 0.3 mg/l (Average specific growth rate)
Based on loading rates

Both test substances are of compositional type A.
**Source:** Palmer and Cann 2000b.
**Test condition:** TEST ORGANISMS
Strain: Raphidocelis subcapitata
Supplier: Institute of Freshwater Ecology, Windermere
Pretreatment: Not reported
Controls: 2 sets of controls (6 replicates and 1 blank flask), one set containing ethanol at 0.1 ml/L
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Ethanol
Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS:
Considered stable

DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0.003, 0.01, 0.03, 0.1, 0.3, and 1 mg/l
Renewal of test solution: None
Exposure vessel type: 287 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 5000 cells/ml
Test temperature: 21.6-23.4
Dissolved oxygen: Not reported
pH mean: 7.7-9.7
Adjustment of pH: None
Intensity of irradiation: Not reported
Photoperiod: Under constant illumination
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION:
At the start and end of the test. Neodol 25E test media concentrations decreased by 40-98% and LIAL 125 test media concentrations decreased by 29-97% over the duration of the test period.

**Test substance:** These results were measured for two similar commercial products, both of compositional Type A.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (32)

**Unit:** mg/l **Analytical monitoring:**

**EC10:** calculated

**EC50:** ca. .1 - 10

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

For compositional Types B and C, for which an estimation of

algal toxicity is required, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type B: 0.1 - 0.3 mg/l
Type C: 1.0 - 10 mg/l

For Type A, a reliable measurement is available, therefore no estimation has been made.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (19)

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = .46
**EbL50 :** = .46 - 1
**ErL50 :** = .46 - 1
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test media was produced using a water accommodated fraction (WAF) methodology and sealed vessels since the material was to be tested at loading rates which exceeded the solubility of some of the components of the mixture.

**Source:** Eadsforth et al. 2000.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but showing greater toxicity are available

11-OCT-2005 (16)

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: biomass and growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EbL50 :** < 1
**ErL50 :** < 1
**Limit Test:** yes

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2001
**GLP:** yes

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Test was carried out with Water accommodated fractions (WAFs), at a loading rate of 1 mg/l, which had been filtered prior to use.
The total measured concentration of the water accommodated fraction of Neodol 25 in test media was 0.26 and 0.24 mg/l at 0 and 72 hours respectively. The mean decrease in levels of the components during the the period of use (72h) was 8%.
**Source:** Palmer and Cann 2001a.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
Not key study: Other studies with same reliability score and showing a range of toxicity are available.
18-JAN-2006 (33)

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EbL0 :** = .3
**EbL50 :** = 2.8
**ErL50 :** = 6.5
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2000
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The test media were produced using a water accommodated fraction (WAF) methodology since the material was to be tested at loading rates which exceeded the solubility of some of the components of the mixture.
**Source:** Henkel KGaA 2000
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but showing greater toxicity are available
11-OCT-2005 (20)

**Species:** other algae: Pseudokirchneriella subcapitata
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = 2.4
**ErL50 :** = 8.7
**EbL50 :** = 5.4
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2003
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** WAFs were prepared by loading test medium with the respective amount of the test item. After stirring the contents were left to settle for 24h. The WAFs were filtered

prior to use through a non polar filter (0.2 um Millex FG, 50 mm, Millipore).
**Source:** Wenzel 2003.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and showing greater toxicity are available
11-OCT-2005 (46)

**Species:** Selenastrum capricornutum (Algae)
**Endpoint:** growth rate
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .4
**Limit Test:** no

**Method:** other
**Year:** 1982
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The acute toxicity of the planktonic alga, Selenastrum capricornutum, was determined in a 4 day growth test. The EC50 value based on growth rate over the period day 0 to day 2 was 0.40 mg/l. This was done as the use of data for day 2 to day 4 would have led to an underestimate of the toxic effects observed.
**Source:** Stephenson 1982b.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and showing greater toxicity are available
11-OCT-2005 (41)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

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## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

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### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

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## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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## 4.6.3 Toxicity to Soil Dwelling Organisms

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## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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## 4.7 Biological Effects Monitoring

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## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in

the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (15)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | other: CD |
| **Sex:** | male/female |
| **No. of Animals:** | 10 |
| **Vehicle:** | other: maize oil |
| **Doses:** | 2000 mg/kg |
| **Value:** | > 2000 mg/kg bw |
| **Method:** | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year:** | 1996 |
| **GLP:** | yes |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: There were no mortalities.<br><br>CLINICAL SIGNS: There were no clinical signs of intoxication. All animals gained bodyweight as expected over the observation period.<br><br>NECROPSY FINDINGS: No adverse effects.<br><br>POTENTIAL TARGET ORGANS: None identified.<br><br>SEX-SPECIFIC DIFFERENCES: NOne |
| **Source:** | Huntingdon Life Sciences Ltd 1996j<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: rat (CD)<br>- Source: Charles River, Margate, Kent, UK<br>- Age: 5 weeks<br>- Weight at study initiation: mean weight prior to fasting males 117-121g, females 108-116g<br>- Group size: 5M+5F<br>- Controls: no<br><br>ADMINISTRATION:<br>- Doses: gavage, animals fasted<br>- Doses per time period: single<br>- Volume administered or concentration: 10 ml/kg in maize oil.<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: The rats were observed twice in the hour immediately after dosing and twice more on the day of dosing. Thereafter the animals were observed twice daily and any observations recorded once a day. Body weights were recorded on days 1, 8 and 15 when the animals were sacrificed. Gross examination was made of the viscera at the end of the observation period. |
| **Test substance:** | Tradename Kalcol 2475 C12-16 alcohols Type B |

**Conclusion:** The rat oral LD50 for Kalcol 2474 is >10g/kg. This dose level had no adverse effect on the test animals.
**Reliability:** (1) valid without restriction
Guideline study.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (25)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 4
**Vehicle:** other: undiluted
**Doses:** 2 and 10 ml/kg
**Value:** > 8300 mg/kg bw

**Method:** other: in house screening procedure
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: None

CLINICAL SIGNS: No signs of toxicity observed.

NECROPSY FINDINGS: Necropsy not carried out.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None
**Source:** Clark & Coombs, 1978
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit
- Age: 12 weeks
- Group size: 2M+2F fasted
- Controls: No

ADMINISTRATION:
- Doses: 2 and 10 ml/kg (specific gravity 0.830)
- Doses per time period: single
- Volume administered or concentration: undiluted
- Post dose observation period: 9 days

EXAMINATIONS: clinical signs, mortality, necropsy was not carried out.
**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A
**Conclusion:** The acute toxicity of Dobanol 25 was determined in rats to be >8300 mg/kg. Rats showed no toxic signs during the observation period.
This study is reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (14) (27)

**Type:** LD50
**Species:** mouse
**Strain:** other: CF1
**Sex:** male

**No. of Animals:** 10
**Vehicle:** water
**Doses:** not reported
**Value:** = 4450 mg/kg bw

**Method:** other: in house screening test
**Year:** 1970
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The mouse oral LD50 for Dobanol 25 was reported to be 4450 g/kg after an 8 day observation period. There were few experimental details in either the summary or original report of this screening study.
**Source:** Henkel, 1970
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A
**Reliability:** (4) not assignable
There were few experimental details in either the summary or original report of this screening study.
25-JUL-2005 (21)

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: undiluted
**Doses:** 5000 mg/kg
**Value:** > 5000 mg/kg bw

**Method:** OECD Guide-line 401 "Acute Oral Toxicity"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived to the end of the 14 day observation period.

CLINICAL SIGNS: None observed. There were no adverse effects on bodyweight.

NECROPSY FINDINGS: None reported

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None.
**Source:** Biolab SGS 1991a
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Nossan-Correzzana, Milan, Italy
- Weight at study initiation: 200g (+- 20 g)
- Group size: 5M+5F
- Controls: yes

ADMINISTRATION: Gavage
- Doses: 5000 mg/kg
- Doses per time period: single (animals fasted)
- Volume administered or concentration: undiluted

- Post dose observation period: 14 days

EXAMINATIONS: Clinical observations made at frequent intervals on the day of dosing then daily. Any decedents and all survivors were necropsied at the end of the observation period. Body weights were recorded at the end of the observation period and compared to controls.

**Test substance:** Tradename Alchem 125 C12-16 alcohols Type A

**Conclusion:** The rat oral LD50 for Alchem 125 is >5000 mg/kg. This dose caused no adverse effects.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (9)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 10
**Vehicle:** other: Condensation mist atmosphere
**Doses:** saturated atmosphere
**Exposure time:** 4 hour(s)

**Method:** other: in house protocol
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 4 hour exposure and subsequent observation period.

CLINICAL SIGNS: There were no signs of toxicity during or after exposure.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None reported.

**Source:** Blair and Sedgwick 1980b
Hayes Consultancy Service Bromley, Kent

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A

**Conclusion:** The 4 hour rat inhalational LC50 for Dobanol 25 is >saturated vapour concentration. There were no signs of toxicity during exposure or the subsequent observation period..

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit, Sittingbourne, Kent, UK
- Age: 8 weeks approx.
- Weight at study initiation: not reported
- Number of animals: 5M+5F
- Controls: none

ADMINISTRATION:
- Type of exposure: 4 hour inhalation exposure, whole body
- Concentrations: saturated atmosphere (no monitoring

reported)
- Particle size: not reported
- Type or preparation of particles: condensation mist

EXAMINATIONS: Clinical signs observed throughout exposure and daily thereafter throughout an observation period of at least 14 days. Initial, 7 and 14 day bodyweights were recorded.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions, no monitoring of saturated atmosphere.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (10)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** male/female
**No. of Animals:** 2
**Vehicle:** other
**Doses:** 830 and 3320 mg/kg
**Value:** > 3320 mg/kg bw

**Method:** other: Noakes and Sanderson, 1969
**Year:** 1969
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the 9 day observation period.

Combined LD50 >3320 mg/kg.

APPLICATION SITE: None reported

CLINICAL SIGNS: No signs of intoxication.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: No.

**Source:** Clark & Coombs, 1978
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: Shell Toxicology Laboratory (Tunstall), Breeding Unit, Sittingbourne, Kent, UK
- Age: 12 weeks
- Group size: 2M+2F
- Controls: No

ADMINISTRATION: 24 hour occluded dermal application
- Area covered: not reported applied to shorn dorsolumbar skin.
- Occlusion: aluminium foil and waterproof plaster.
- Vehicle: undiluted
- Total volume applied: ca 4 ml/kg
- Doses: 1 and 4 ml/kg (830 and 3320 mg/l using the specific gravity reported of 0.83)

- Removal of test substance: washed with tepid dilute detergent solution.

EXAMINATIONS: Mortality and clinical signs during the 9 day observation period.

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A

**Conclusion:** Rat dermal LD50 >3320 mg/kg (24 hour occluded). There were no signs of toxicity.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.

**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** other: New Zealand White rabbit

**Concentration:** 100 %

**Exposure:** Occlusive

**Exposure Time:** 4 hour(s)

**No. of Animals:** 6

**Vehicle:** other: undiluted

**Result:** slightly irritating

**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"

**Year:** 1991

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual mean 24+48+72 hour scores 4 rabbits scored 1, 2 rabbits scored 1.7 (Group mean 24+48+72 hour score 1.2)
- Oedema: All rabbits scored 1 at 24, 48 and 72 hours. The group mean and individual scores are therefore 1.

REVERSIBILITY: Erythema and oedema persisted throughout the 7 day observation period in all animals (grade 1). Group mean scores at 5 and 7 days were 1 for both erythema and oedema.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS 1991
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported

- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy
- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Alchem 125 C12-16 alcohols Type A
**Conclusion:** Following a 4 hour occluded exposure to rabbit skin Alchem 125 considered as non-irritant by EU criteria and a mild irritant by GHS (class 3).
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (8)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1984
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual 24+48+48 hours scores were 1 in 4 rabbits and 0.7 in 2 rabbits. (Group mean 24+48+72 hour score 0.9)
- Edema: All scores were 0.

REVERSIBILITY: All scores were 0 by observation day 5.

OTHER EFFECTS: None reported.

**Source:** Biolab SGS, 1984d
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: not reported
- Source: Padre Antonio Breeding Centre, Mariano Comense, Italy

- Weight at study initiation: 2-3 kg
- Number of animals: 6
- Controls: not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 6x6 cm
- Occlusion: Occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 7 days
- Removal of test substance: with water or appropriate solvent.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours, 5 and 7 days.

**Test substance:** Tradename Lial 125 C12-16 alcohols Type A
**Conclusion:** Following a 4 hour occlusive exposure Lial 125 was not irritating to rabbit skin using EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (7)

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 8
**Vehicle:** other: undiluted
**PDII:** 4
**Result:** irritating
**EC classificat.:** irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE
- Erythema: Individual mean 24+72 hour scores abraded skin 2.5, 2.3, 1.8, 3.0 (group mean 24+73 hour score 2.4); intact skin 1.8, 2.5, 2.3, 2.5 (group mean 24+73 hour score 2.3)
- Edema: Individual mean 24+72 hour scores abraded skin 1.3, 1.5, 0.8, 1.5 (group mean 24+73 hour score 1.8); intact skin 2, 1.3, 1.5, 1.8 (group mean 24+73 hour score 1.7)

REVERSIBILITY: The irritation persisted throughout the 7 days observation period with group mean erythema scores for abraded and intact skin of 1.5 and 0.8 respectively and oedema scores abraded and intact skin of 1.4 and 0.6 respectively.

OTHER EFFECTS: None reported.

**Source:** Clark & Coombs, 1978
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: female
- Source: Shell Toxicology Breeding Laboratory, Sittingbourne,

UK
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 8 (2M+2F abraded skin, 2M+2F intact skin.
- Controls: Not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: 2x2 cm
- Occlusion: occluded
- Vehicle: None
- Total volume applied: 0.5 ml
- Exposure period: 24 hours to intact and abraded skin.
- Postexposure period: 7 days
- Removal of test substance: Washed with warm dilute detergent solution.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours and at 7 days.

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A

**Conclusion:** Following 24 hour occlusive application Dobanol 25 was irritant to intact and abraded rabbit skin when assessed using both EU and GHS criteria based on a group mean 24+72 hour score of 2.4 or 2.3 for erythema with 2 individual animal scores >=2.3 and persistance to the end of the observation period.

Study reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14) (27)

**Remark:** Unpublished data ex Henkel:
Archive RT.920070 as reported in Iuclid 2000 Rabbit skin irritation test according to OECD 404 test substance but exposure time and method of occlusion not detailed. Described as an EU irritant. No further details available.

**Test substance:** As prescribed in 1.1 - 1.4.
Insufficient compositional details to ascribe to a type.

**Reliability:** (4) not assignable
Secondary reference to unpublished data.

25-JUL-2005 (27)

**Species:** other: New Zealand White rabbit
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 3
**Vehicle:** water
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE

- Erythema: Individual 24+48+72 hour scores 1.0, 1.0, 1.7 (group mean score 1.2)
- Oedema: All scores 0.

All control sites were normal and showed no skin irritation.

REVERSIBILITY: Erythema and/or oedema persisted in one animal only until observation day 10. All scores were 0 on days 13 and 16.

OTHER EFFECTS: Exfoliation was observed in two test animals on days 13 and 16.

**Source:** Johnson 1996c
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: ca 3 months
- Weight at study initiation: 2.22 - 2.64 kg
- Number of animals: 3

ADMINISTRATION/EXPOSURE
- Preparation of test substance: The test material was a white solid, the test site was mositened with 0.2 ml purified water prior to application of 0.5 g of the solid.
- Area of exposure: 3X2 cm
- Occlusion: semi-occlusive
- Vehicle: None
- Total volume applied: 0.5 g
- Exposure period: 4 hours
- Postexposure period: 16 days
- Controls: The other flank of the animal was used as a control site.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours post application then at 7, 10, 13 and 16 days.

**Test substance:** Tradename Kalcol 2475 C12-16 alcohols Type B

**Conclusion:** Following a 4 hour semi-occlusive exposure undiluted Kalcol 2475 was not irritating to rabbit skin when classified by EU or GHA criteria. The group mean score for erythema was 1.2. A score greater than 1.5 was observed in one animal only.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (29)

**Remark:** Unpublished data ex Henkel:
Archive R 9700781 (as reported in Iuclid 2000) Human skin irritation assay using the Burckhardt method, 1970. Result not irritating. No further details available.

**Test substance:** As prescribed in 1.1 - 1.4.
Insufficient compositional details to ascribe to a type.

**Reliability:** (4) not assignable
Secondary reference to unpublished data.

25-JUL-2005 (27)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Directive 84/449/EEC, B.5 "Acute toxicity (eye irritation)"
**Year:** 1991
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: Group mean score 0
- Iris: Group mean score 0
- Conjunctivae (Redness): Group mean score 0.6
- Conjunctivae (Chemosis): Group mean score 0

REVERSIBILITY: All scores were 0 at day 7.

Individual scores were not available.
**Source:** Biolab SGS 1991h
Hayes Consultancy Service Bromley, Kent
**Test condition:** Summary data only provided.
**Test substance:** Tradename Alchem 125 C12-16 alcohols Type A
**Conclusion:** From the limited data available Alchem 125 is not considered an eye irritant according to EU or GHS criteria.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
25-JUL-2005 (6)

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .2 ml
**Comment:** not rinsed
**No. of Animals:** 4
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0.27
- Conjunctivae (Chemosis): 0.17

Individual scores were not reported.

REVERSIBILITY: Scores for all parameters 0 by day 2 (48 hours

post instillation) and continued 0 until day 7.

OTHER EFFECTS: There was no discharge.

**Source:** Clark & Coombs, 1978
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: rabbit
- Strain: New Zealand White
- Sex: not reported
- Source: Shell Toxicology Laboratory (Tunstall) Breeding Unit.
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 4
- Controls: Untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.2 ml
- Vehicle: none
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: not reported
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: Not reported

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A

**Conclusion:** Dobanol 25 is not an eye irritant according to EU or GHS criteria.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14) (27)

**Species:** other: New Zealand White rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 3
**Vehicle:** other: applied as a solid
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: All scores 0
- Iris: All scores 0
- Conjunctivae (Redness): Individual scores 0.7, 0, 0.3 (group mean score 0.33)
- Conjunctivae (Chemosis): All scores 0

DESCRIPTION OF LESIONS: Iritis and/or slight conjunctivitis and discharge was observed during the first hour following instillation. Scores for all parameters for all 3 animals were 0 at 24 hours. In 2 animals slight conjunctivitis appeared at

48 or 72 hours with discharge in one animal at 72 hours. The treated eye of the remaining rabbit was overtly normal by day 2 and remained normal.

REVERSIBILITY: Slight conjunctival redness (grade 1, some vessels definitely injected) persisted in two animals until the end of the study (day 22) although one of these animals scored 0 at day 8, then 1 at days 15 and 22. One rabbit was scored 1 for iritis on day 15.

OTHER EFFECTS: Instillation of the test material caused no initial pain response.

**Source:** Johnson 1996f
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: female
- Source: Froxfield SPF Rabbits, Hampshire, UK
- Age: 5 months
- Weight at study initiation: 2.63 - 2.99 kg
- Number of animals: 3
- Controls: untreated eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the test material was a white solid and applied as received from the supplier.
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 22 days

EXAMINATIONS
- Scoring system: As prescribed in OECD test method.
- Observation period: 22 days
- Tool used to assess score: Ophthalmoscope or pencil beam tourch.

**Test substance:** Tradename Kalcol 2475 C12-16 alcohols Type B

**Conclusion:** The results of this study indicate a minimal initial response to the test material. However there was persistence of this minimal response in a rather intermittent pattern in 2 test animals. Kalcol 2475 is not considered to be classifiable as an eye irritant by either EU or GHS criteria.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (30)

## 5.3 Sensitization

**Type:** Guinea pig maximization test
**Species:** guinea pig
**Concentration 1st:** Induction .1 % intracutaneous
**2nd:** Induction 5 % occlusive epicutaneous
**3rd:** Challenge 2.5 % occlusive epicutaneous
**No. of Animals:** 20
**Vehicle:** other: corn oil
**Result:** not sensitizing
**Classification:** not sensitizing

**Method:** other: M&K guinea pig maximzation test

**Year:** 1978
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS OF PILOT STUDY: No details given.

RESULTS OF TEST
- Sensitization reaction: 0/20 treated, 0/10 controls at 24 and 48 hours, result negative.
- Clinical signs: None in test or controls.
- Rechallenge: Not carried out.

**Test condition:** TEST ANIMALS: Guinea pig
- Strain: P-strain
- Sex: male & female
- Source: Shell Toxicology Lab (Tunstall) breeding unit.
- Age/weight: Not reported
- Number of animals: 10M+10F
- Controls: 5M+5F

ADMINISTRATION/EXPOSURE
- Study type: Maximization (M&K)
- Preparation of test substance for induction: In corn oil
- Preparation of test substance for challenge: In corn oil
- Induction schedule: Intradermal injection followed one week later by topical application (48 hours occlusive).
- Concentrations used for induction: 0.1% intradermal, 5% topical.
- Concentration in Freuds Complete Adjuvant (FCA): no data
- Challenge schedule: 2 weeks after topical induction, 24 hour topical challenge.
- Concentrations used for challenge: 2.5% in corn oil.
- Rechallenge: No
- Positive control: Not reported

EXAMINATIONS
- Grading system: 4 point scale -ve, trace, +ve, ++ve.
- Pilot study: Initial irritation screen, no details given.

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A
**Conclusion:** Dobanol 25 was not a skin sensitiser in guinea pigs when tested using the M&K maximization assay. Reported in Iuclid 2000.
**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.
**Flag:** Critical study for SIDS endpoint
05-DEC-2005 (14) (27)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C12-16 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), 1-hexadecanol and C18 (octadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (38) (39) (44)

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** other: Bacterial reverse mutation assay (Ames test)
**System of testing:** Salmonella typhimurium strains TA98 and TA100
**Concentration:** 5 to 500 ug/plate
**Cytotoxic Concentration:** 500 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** other: Ames
**Year:** 1996
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation:
- Preliminary screen: absence of revertant colonies at 2500 and 5000 ug/plate with absence or thinning of background lawn, slight thinning of background lawn at 500 ug/plate, lower dose levels not cytotoxic.
- Main study: No increase in reverse mutation rate compared to controls at any concentration tested. Postive controls showed appropriate increases in reverse mutation rate.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
With and without metabolic activation: Slight thinning of bacground lawn and decreased reversion rate at 500 ug/plate (top dose level tested).

**Source:** Huntingdon Life Sciences Ltd 1996m.

Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA98 and TA100
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arocholor 1254 induced.

ADMINISTRATION:
- Dosing: 5, 15.8, 50, 158, 500 ug/plate based on preliminary toxicity testing in TA98 at dose levels ranging from 2.5-5000

ug/plate..
- Number of replicates: Duplicate
- Application: Pour plate, solvent DMSO.
- Positive and negative control groups and treatment: Negative controls DMSO and untreated bacterial control. Positive controls benzo[a]pyrene 5 ug/plate, sodium azide 2 ug/plate, 2-nitrofluorene 1 ug/plate.
- Incubation: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: not reported

**Test substance:** Tradename Kalcol 2475 C12-16 alcohols Type B

**Conclusion:** The C12-16 alcohol Kalkohl 2475 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to and including 500 ug/plate. Evidence of cytotoxicity was observed at 5000 ug/plate (highest dose level tested).

**Reliability:** (2) valid with restrictions
Ames test no protocol specified but similar OECD 471 using only 2 tester strains. Criteria for evaluation were not reported.

**Flag:** Critical study for SIDS endpoint

11-MAY-2006 (26)

**Type:** other: Bacterial reverse mutation assay (Ames Test)
**System of testing:** Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 102
**Concentration:** 1.25 to 200 ug/plate
**Cytotoxic Concentration:** Varies with the strain 10 - 1000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** GENOTOXIC EFFECTS:
- With and without metabolic activation: No increased incidence of reverse mutations at any dose levels tested, positive controls showed an appropriate increase in mutations.

PRECIPITATION CONCENTRATION: Precipitation observed at 1000 ug/plate and above.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: There was variability in the toxic response of the various tester strains to Dobanol 25. As a result in the second experiment various additional dose levels were added. Strain TA 1537 was particularly sensitive and slight toxicity was observed at 10 ug/plate. There was no obvious toxicity with TA 1535 up to 1000 ug/plate although slight toxic effects may have been obscured by precipitation at this level and above. Toxic effects were seen in TA98 and 100 with S9 at 250 ug/plate and with TA102 at 62.5 +S9 and at 250 -S9. It was concluded that a sufficient number of dose levels were assessed where toxicity did not confound the result.

**Source:** Ballantyne 1996.

Hayes Consultancy Service Bromley, Kent

**Test condition:** SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 102
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced. Activity checked by supplier.

ADMINISTRATION:
- Dosing: Experiment 1: 0, 8, 40, 200, 1000, 5000 ug/plate. Experiment 2: between 1.25 and 200 ug/plate depending on toxicity.
- Number of replicates: Triplicate
- Application: Experiment 1: Plate incorporation; Experiment 2: Preincubation for tests with metabolic activation.
- Positive and negative control groups and treatment: Negative controls, solvent (DMSO) and untreated bacteria. Postive controls sodium azide 2 ug/plate, 2-aminoanthracene 5 ug/plate, 9-aminoacridine 50 ug/plate, 2-nitrofluorene 50 ug/plate, glutaraldehyde 25 ug/plate.
- Incubation time: 72 hours at 37C
- Preincubation time: 1 hour at 37C

CRITERIA FOR EVALUATING RESULTS: Considered to be mutagenic if test was valid and reproducible and Dunnetts test gave a positive response ($p<0.01$) with a significant dose correlation.

**Test substance:** Tradename Dobanol 25 C12-16 alcohols Type A

**Conclusion:** The C12-16 alcohol Dobanol 25 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels including those which showed some degree of cytotoxicity.

**Reliability:** (1) valid without restriction
Guideline study.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (5)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol, dodecanol, C12-16 (types A & B), C12-18 (type B), tetradecanol, hexadecanol and octadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
14-SEP-2005 (38) (39) (44)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C12-16 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexadecanol) and data from supporting substances 1-hexanol-2-ethyl, isoamyl alcohol and C18 (octadecanol).
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (38) (39) (44)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C12-16 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (38) (39) (44)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

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(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

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(19) Fisk, P.R et al, 2005: Ecotoxicology: Interpretation of data for multi-component substances; Annex IV to the Long Chain Alcohols SIAR.

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# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 75782-86-4
**CAS No.** 75782-86-4
**EINECS Name** Alcohols, C12-13
**EC No.** 278-306-0

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
**Revision date:**
**Date of last Update:** **29-DEC-2005**

**Number of Pages:** **41**

**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

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04-AUG-2005

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**Remark:** Industry Consortium
23-AUG-2005

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**Type:** cooperating company
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**Remark:** Consortium Member
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**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C12-13 alcohols, CAS 75782-86-4 are >80% linear.

The substance comprises >95% C12 and 13. Components of even and odd chain length, in the range C11-C15 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required

11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C12-13 (CA INDEX NAME)
Alchem 123
C12-13 alcohols
Dobanol 23
Neodol 23
Neodol 23-6.8
Neodol R 23
Oxocol 1213
Safol 23

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C12-13 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >50 000 - 250 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to >100 000 000 - 500 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (5) (8) (14)

## 1.6.1 Labelling

**Remark:** Not required

11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

-

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-13 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

## 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
11-AUG-2003

## 2.1 Melting Point

**Value:** 25 degree C

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
**Reliability:** (2) valid with restrictions
23-AUG-2005

## 2.2 Boiling Point

**Value:**

**Remark:** The substance has a range of components, as described in section 1.1-1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (13)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00083 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (1)

**Value:** < .1 hPa at 25 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
This information was obtained from secondary literature (company product data) and cannot be validated further.
11-OCT-2005 (11)

## 2.5 Partition Coefficient

**log Pow:** = 5.4 - 5.5 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
19-SEP-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 1.1 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a

standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The water solubility is estimated to be 1.1 mg/l at a loading rate of 1000 mg/l.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

15-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.

**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.

**Flag:** Critical study for SIDS endpoint
06-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure).

Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:**

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 36600 |
| Non-hydrophobics method: | Koc = 6420 - 7680 |
| TGD Alcohols method: | Koc = 390 - 450 |
| SRC PCKOCWIN method: | Koc = 330 - 600 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

21-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 4500 - 9600

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = .58 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .49 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty

alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (6)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** other: reported as albino rats
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other:undiluted
**Doses:** 10.25, 15,38, 23.07 and 34.6 g/kg
**Value:** =

**Method:** other: contract laboratory protocol
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All occurred within 2-3 days of dosing.
- Number of deaths at each dose: 0/4, 0/4, 0/4, 4/4

Acute oral LD50 28.2 g/kg (standard deviation 1.5 g)

CLINICAL SIGNS: All rats at the 3 higher dose levels exhibited lethargy and/or generalised weakness this was classed as moderate at 15.38 g/kg with an onset within 60-90 minutes. At the two top dose levels the reaction was classed as severe with an onset within 30 minutes of dosing. All survivors had recovered by day 5.
Rats at the top two dose levels exhibited wet fur over the entire body reportedly due to transfer of fluid through the skin. All survivors had recovered by day 5.

NECROPSY FINDINGS: There were no significant findings among survivors. Among premature decedents (top dose only) blood was present in the stomach 3/4 and small intestine (1/4). Ulcerated areas were observed in the pyloric region of the stomach (2/4) and petechial haemorrhages also in the pyloric stomach (1/4).

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: None observed.
**Source:** Shell, 1966
**Test condition:** TEST ORGANISMS: rat (albino)
- Source: no reported
- Age: young adults
- Weight at study initiation: 94-120g
- Group size: 2M+2F (fasted)
- Controls: No

ADMINISTRATION: gavage

- Doses: 10.25, 15.38, 23.07 and 34.6 g/kg
- Doses per time period: not reported
- Volume administered or concentration: undiluted
- Post dose observation period: 14 days

EXAMINATIONS: Mortality and clinical signs were observed over the 14 day observation period. All animals were subject to gross necropsy either at time of death or at the end of the observation period.

**Test substance:** Tradename Neodol 23CG

**Conclusion:** The rat oral LD50 for Neodol 23CG is 28.2 g/kg. Clinical signs were confined to lethargy and generalised weakness. In premature decedents gross necropsy revealed ulceration and haemorrhaging of the gastric mucosa.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (10)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C10 (1-decanol), C12 (1-dodecanol), C12-16, C14 (tetradecanol), tridecanol (Cas 112-70-9), C14 (tetradecanol) and C16 (hexadecanol) alcohols in support of the statement that C12-13 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (12) (15)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: undiluted test material
**Doses:** 6.834, 10,25, 15.38 and 23.07 g/kg
**Value:** = 11300 mg/kg bw

**Method:** other: Contract laboratory protocol
**Year:** 1966
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY:
- Time of death: All animals died within 1-9 days of exposure
- Number of deaths at each dose: 0/4, 2/4, 3/4, 4/4.

LD50 (M+F) 11.3 g/kg (standard deviation +- 2.2 g/kg)

APPLICATION SITE: By the end of the exposure period all rabbits exhibited erythema at the application site ranging from mild to severe. The recovery time for all surviors was up to day 8. Drying of theskin and sunsequent fissuring with loss of uppermost layers developed from day 4 and continued to the end of the observation period.

CLINICAL SIGNS: Anorexia was observed in all animals continuing throughout the observation period at the two mid-dose levels and until day 3 at the low dose (all top dose animals died). Generalised weakness was observed in all but 1 low dose rabbit within 2-20 hours of dosing. Low dose animals recovered during the observation period while in the mid dose animals this condition persisted until the end of the observation period.
Oily fur reportedly due to transfer of fluid through the skin was observed in all treated animals recovery occurred in 5 days (low dose, 7-9 days 10.25 g/kg) and continued through the observation period at 15.38 g/kg. Some animals at the 3 higher dose levels exhibited iritis within 0-2 days of dosing and clearing within 3-5 days.

NECROPSY FINDINGS: There were no remarkable findings among survivors. In premature decedents hyperemic lungs and thickening of the skin at the application site were reported.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: No significant difference.

**Source:** Shell 1966
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: not reported
- Age: young adult
- Weight at study initiation: 2.6-3.4 kg
- Group size: 2M+2F
- Controls: no

ADMINISTRATION: 24 hour occluded application to intact skin.
- Area covered: 10% body area clipped.
- Occlusion: plsatic film secured with adhesive tape.
- Vehicle: undiluted
- Concentration in vehicle:
- Total volume applied:
- Doses: 6.834, 10,25, 15.38 and 23.07 g/kg
- Removal of test substance: not reported

EXAMINATIONS: Mortality and clinical signs of toxicity and skin irritation were observed throughout the 14 day observation period. gross necropsy was carried out on all rabbits either at the time of death or at the end of the observation period.

**Test substance:** Tradename Neodol 23CG

**Conclusion:** The rabbit dermal LD50 (24 hour occluded) for Neodol 23CG was

11.3 g/kg. Persistent skin irritation was noted at the application site of most rabbits. Clinical signs of intoxication were anorexia and generalised weakness. Oily fur was observed in all animals. Findings at gross necropsy were unremarkable in survivors. The main findings in premature decedents were hyperaemic lungs and thickening of the skin at the applicaton site.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (10)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**PDII:** 2.37
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+72 hour mean
- Erythema: Intact skin 1.83, Abraded skin 1.83
- Oedema: Intact skin 0.5, Abraded skin 0.59
Individual scores were not reported. PII 2.37

REVERSIBILITY: Based on mean scores erythema had not regressed by 72 hours while there was a slight reduction in mean oedema scores.

OTHER EFFECTS: None reported.

**Source:** Shell, 1966
**Test condition:** TEST ANIMALS: Rabbits (albino)
- Sex: Not reported.
- Source: Not reported.
- Age: Not reported.
- Weight at study initiation: Not reported.
- Number of animals: 6

- Controls: No

ADMINISTRATION/EXPOSURE 24 administration to intact and abraded skin.
- Preparation of test substance: Undiluted
- Area of exposure: 2X2 inches
- Occlusion: Occlusive
- Vehicle: Undiluted
- Total volume applied: 0.5 ml
- Postexposure period: 72 hours
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours

**Test substance:** Tradename Neodol 23CG

**Conclusion:** Based on the limited data available it is not considered that Neodol 23CG undiluted is a skin irritant in a 24 hour Draize test according to EU criteria. In the absence of individual animal scores it is not possible to accurately classify according to GHS criteria however it is likely that Neodol 23CG would be at most a mild skin irritant based on this classification system.

**Reliability:** (2) valid with restrictions
Study method well documented however individual animal results not reported. Meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (10)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 5
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE (24+48+72 hour)
- Cornea: 0
- Iris: 0
- Conjunctivae (Redness): 0
- Conjunctivae (Chemosis): 0
- Overall irritation score: 0

DESCRIPTION OF LESIONS: Conjunctival redness and/or oedema was observed in 3/5 eyes at 1 hour after instillation.

REVERSIBILITY: All eyes appeared normal by 24 hours after instillation and remained normal until the end of the 7 day observation period.

OTHER EFFECTS: None reported.

**Source:** Shell, 1966

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported.
- Source: Not reported.
- Age: Young adults.
- Weight at study initiation: Not reported
- Number of animals: 5
- Controls: The untreated eye served as a control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: Not reported.
- Scoring system: Draize
- Observation period: 7 days
- Tool used to assess score: None mentioned.

**Test substance:** Tradename Neodol 23CG

**Conclusion:** Neodol 23 CG is not an eye irritant according to EU or GHS criteria. Group mean 24+48+72 hour scores were 0.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (10)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A), C14 (tetradecanol) and C16 (hexadecanol) alcohols which support the conclusion that C12-13 alcohols are not expected to be skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

05-DEC-2005 (12) (15)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C12-13 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type B) and 1-hexadecanol . The oral NOAELs for these studies are

all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (12) (15)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C12-13 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, tetradecanol and hexadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

14-SEP-2005 (12) (15)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol, dodecanol, C12-16 (types A & B), C12-18 (type B), tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting)

[negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
14-SEP-2005 (7) (12) (15)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C12-13 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14 -16 (type A) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (7) (9) (12) (15)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C12-13 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of

maternal toxicity.

**Reliability:** (2) valid with restrictions
14-SEP-2005 (9) (12) (15)

### 5.8.3 Toxicity to Reproduction, Other Studies

-

### 5.9 Specific Investigations

-

### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(5) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(6) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(7) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(8) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(9) Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(10) Shell, 1966. Acute toxicity studies on NEODOL 23 CG. Shell proprietary report HSE-66-0061.

(11) Shell. 2000d. Shell Chemical Company NEODOL product guide.

(12) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(13) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(14) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(15) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 75782-87-5
**CAS No.** 75782-87-5
**Substance name** Alcohols, C14-15

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
**Revision date:**
**Date of last Update:** **18-JAN-2006**

**Number of Pages:** **40**

**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
**Street:** Evenlode House, Howbery Park
**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

23-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
**Street:** Vaarstraat 130
**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
**Street:** 1 Paul-Baumann-Strasse
**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20057 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.
The individual substances covered by the Long Chain Alcohols Category are:

| Chemical name | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |

| | |
|---|---|
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C14-15 alcohols, CAS 75782-87-5 are >80% linear.

The substance comprises >95% C14 and 15. Components of even and odd chain length, in the range C12-C17 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C14-15 (CA INDEX NAME)
Alchem 145
Dobanol 45
Neodol 45
Neodol 45E
OX 1415
Oxocol 1415

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C14-15 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

USA: ca. >50 000 - 250 000 tonnes (CAS-specific data) - This is the publicly-available US IUR quantity (i.e. total production plus import) for USA, for 2002. This is equivalent to 100 000 000 - 500 000 000 pounds.

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (5) (9) (13)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

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### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

-

### 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 656 and 3532
05-AUG-2005 (15)

## 1.8.4 Major Accident Hazards

-

## 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

-

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C14-15 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
04-AUG-2005

## 2.1 Melting Point

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
**Reliability:** (2) valid with restrictions
21-OCT-2005

## 2.2 Boiling Point

**Value:**

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.
21-OCT-2005

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (12)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00011 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has

been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 6 - 6.4

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
11-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .15 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The water solubility is estimated to be 0.15 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 96500 - 203000 |
| TGD Non-hydrophobics method: | Koc = 14300 - 23100 |
| TGD Alcohols method: | Koc = 711 - 1020 |
| SRC PCKOCWIN method: | Koc = 1110 - 2050 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: calculated (read across from other measured results)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window, based on results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 24000 - 42600

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.
The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.
29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = .29 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

## 4.6.2 Toxicity to Terrestrial Plants

-

## 4.6.3 Toxicity to Soil Dwelling Organisms

-

## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

-

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a

series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (6)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | other: reported only as albino rats |
| **Sex:** | male/female |
| **No. of Animals:** | 12 |
| **Vehicle:** | other: 50% in corn oil and undiluted (top dose) |
| **Doses:** | 15.38, 23.07 and 34.6 g/kg |
| **Value:** | > 23100 mg/kg bw |
| **Method:** | other: contract laboratory protocol |
| **Year:** | 1966 |
| **GLP:** | no |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY:<br>- Time of death: 4-17 hours after doing for animals administered the material in corn oil. The single animal which died following dosing with undiluted material died on day 2 after dosing.<br>- Number of deaths at each dose: 0/4, 1F/4, 2M/4 (1F/4 tested undiluted)<br><br>CLINICAL SIGNS: All animals displayed mild (lowest dose) to severe inactivity and generalized weakness within 1-20 hours of dosing. These symptoms disappeared within 2 (low dose) to 4 days. Wet fur (moderate to severe), reportedly indicative of a transfer of large amounts of fluid through the skin, was observed within 4-20 hours of dosing in all except the lowest dose level animals and persisted until day 4.<br><br>NECROPSY FINDINGS: In one decedent receiving the top dose level in corn oil the presence of solidified material was noted in the stomach. The lungs of one decedent in each of the top dose groups (in corn oil and undiluted) were reported as hyperemic. Blood was observed in the small intestine of the animal which died after receiving the high dose level undiluted. Gross findings in survivors were unremarkable.<br><br>POTENTIAL TARGET ORGANS: None identified.<br><br>SEX-SPECIFIC DIFFERENCES: No clear differences. |
| **Source:** | Lifestream Laboratories 1966<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS: Albino rats<br>- Source: not reported<br>- Weight at study initiation: 93-121g<br>- Group size: 2M+2F fasted<br>- Controls: no |

ADMINISTRATION: Gavage
- Doses: 15.38, 23.07 and 34.6 g/kg
- Doses per time period: not reported
- Volume administered or concentration: Adminstered as a 50% solution in corn oil additionally the top dose level was administered undiluted.
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for clinical signs of toxicity and mortality. All decedents and survivors were subject to gross necropsy.

**Test substance:** Tradename Neodol 45

**Conclusion:** The rat oral LD50 for Neodol 45 was in excess of 23.07 g/kg. Insufficient animals died at the top dose level to calculate a true LD50 value. The signs of intoxication were confined to lethargy and generalised weakness and wet fur. All animals were normal within 4 days of dosing.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (8)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C12 (1-dodecanol), C12-16, C14 (tetradecanol) and C16 (hexadecanol) alcohols in support of the statement that C14-15 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (14)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male/female
**No. of Animals:** 16
**Vehicle:** other: 50% w/v solution of Neodol 45 in Dowanol DPM
**Doses:** 3.038, 4.556, 6.834 and 10.25 g/kg
**Value:** = 6180 mg/kg bw

**Method:** other: Contract laboratory protocol
**Year:** 1966

**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: Total 7/16
- Time of death: 4 rats died during the exposure period, 3 others died between days 3 and 6.
- Number of deaths at each dose: 0/4, 1/4, 2/4, 4/4

LD50 (M+F) 8.18 g/kg (standard deviation 0.96 g/kg) The dermal LD50 of Dowanol DPM was reported to be greater than 20 ml/kg.

APPLICATION SITE: Erythema (mild -severe) was observed at the application site within 24 hours, with recovery in survivors by day 8. Within 1-2 days there was drying of the site and subsequent fissuring with loss of the uppermost layers which continued throughout the observation period.

CLINICAL SIGNS: General weakness was observed in 10 rabbits within 24 hours with recovery between days 2 and 5. Anorexia was observed in all rabbits, recovery of survivors occurred between days 5-7. Iritis was observed 10 rabbits within 24 hours reversing between days 2 and 4.

NECROPSY FINDINGS: There were no remarkable gross pathological findings amongst survivors. In premature decedents hyperaemic lungs were observed in all animals. Thickening of skin at the application site was observed in most decedents.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: No conclusion drawn.

**Source:** Lifestream Laboratories 1966
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported
- Age: Young adults
- Weight at study initiation: 2.5-3.5 kg
- Group size: 2M+2F intact skin
- Controls: no

ADMINISTRATION: 24 hour occluded exposure
- Area covered: 10% of body surface clipped for application.
- Occlusion: Plastic film
- Vehicle: Dowanol DPM
- Concentration in vehicle: 50%
- Total volume applied:
- Doses: 3.038, 4.556, 6.834 and 10.25 g/kg
- Removal of test substance: Not reported.

EXAMINATIONS: Periodic examination for mortality and clinical signs during exposure then daily thereafter including monitoring for skin irritation at the application site. All animals were subject to gross necropsy.

STATISTICAL METHODS: The LD50 was calculated using the methods of Weil 1952 and Thompson et al, 1947 and 1952.

**Test substance:** Tradename Neodol 45

**Conclusion:** The rabbit dermal LD50 for Neodol 45 as a 50% solution in Dowanol DPM was 6.18 g/kg. Skin irritiation was observed at the application site of all animals persisting until the end

of the observation period. Clinical signs of toxicity were generalised weakness and anorexia. Iritis was reported during exposure peristing for several days. Findings at gross necropsy were unremarkable for survivors.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (8)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** 50 %
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** other: Dowanol DPM
**PDII:** 2.2
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE: The scores were presented as combined erythema and oedema scores for individual rabbits for intact and abraded skin. It is not possible to present the data in an EU/GHS format. The test material is described as mildly irritating with a Primary Irritation Rating of 2.2 (max. 8)

REVERSIBILITY: Skin irritation was still present at 72 hours.

OTHER EFFECTS: Not reported.

**Source:** Lifestream Laboratories, 1966
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: Albino
- Sex: Not reported.
- Source: Not reported.
- Age: Not reported.
- Weight at study initiation: Not reported.
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour occlusive application to intact and abraded skin.
- Preparation of test substance: As a 50% solution
- Area of exposure: 2 inch square.
- Occlusion: Occlusive
- Vehicle: 50% in Dowanol DPM
- Total volume applied: 1 ml
- Postexposure period: 72 hours
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours after exposure.

**Test substance:** Tradename Neodol 45

**Conclusion:** Neodol 45 is considered mildly irritating according to the Draize scoring system with a PII of 2.0, following a 24 hour occlusive application to rabbit skin. It is considered that this degree of irritation in a Draize test would not trigger classification according to EU criteria and would at most suggest a GHS classification as a mild irritant.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (8)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 5
**Vehicle:** other: gentle warming to liquify.
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1966
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE The scores were reported as prescribed by the FDA 1959. Although individual animal data are provided only the converted scores are reported so it is not possible to present the data according to EC/GHS criteria. The average score (includes all end points) for each time point was as follows:

1 hour: 2.4; 24 hours: 0.8
All other time points up to 7 days scored 0 for all parameters.

DESCRIPTION OF LESIONS:
- Cornea: There were no corneal effects, all scores were 0.
- Iris: There was no effect on the iris, all scores 0.
- Conjunctivae (Redness and chemosis): Redness and/or chemosis was observed in 4/5 eyes at 1 hour and in 2/5 eyes at 24 hours

post instillation. Scores at all other time points were 0.

REVERSIBILITY: The slight effects on the conjunctivae at 1 and 24 hours post instillation were completely reversed by 48 hours. All eyes continued normal until the end of the observation period.

OTHER EFFECTS: None reported.

**Source:** Lifestream Laboratories, 1966
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Not reported.
- Source: Not reported.
- Age: Young adults
- Weight at study initiation: Not reported.
- Number of animals: 5
- Controls: The untreated eye served as a control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted, Neodol 45 is a solid and it was warmed gently to liquify before instillation into the eye.
- Amount of substance instilled: 0.1 ml
- Vehicle: undiluted
- Postexposure period: 7 days

EXAMINATIONS
- Ophthalmoscopic examination: Not reported.
- Scoring system: Draize
- Observation period: at 1, 2, 3, 4 and 7 days.
- Tool used to assess score: Not reported.

**Test substance:** Tradename Neodol 45

**Conclusion:** Neodol 45 applied undiluted to the rabbit eye is not classifiable as an eye irritant by either EU or GHS criteria. Although scores are not presented in the EU format it is obvious that the degree of irritation observed would not trigger classification.

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (8)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon r, all assays were negative. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A), C14 (tetradecanol), C14-16 (Type A) and C16 (hexadecanol) alcohols which support the conclusion that C14-15 alcohols are not expected to be skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

05-DEC-2005 (10) (14)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C14-15 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), C16 (1-hexadecanol) and C18 (octadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5- to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C14-15 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests

over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, C12-16 (types A&B), tetradecanol, hexadecanol and octadecanol [Ames].

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (7) (10) (11) (14)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C14-15 alcohols (tetradecanol) are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving C10-16 alcohols (types B&D), C14-16 (type A) and C16 (hexadecanol) and from the supporting substance C18 (octadecanol).

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C14-15 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (11) (14)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(5) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(6) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(7) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(8) Lifestream Laboratories. 1966. Acute toxicity studies on NEODOL 45.

(9) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(10) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(11) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(12) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(13) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(14) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(15) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 80206-82-2
**CAS No.** 80206-82-2
**EINECS Name** Alcohols, C12-14
**EC No.** 279-420-3

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
**Revision date:**
**Date of last Update:** **30-DEC-2005**

**Number of Pages:** **54**

**Chapter (profile):** Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
**Name:** UK The Environment Agency
**Contact Person:** Steve Dungey **Date:**
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**Town:** OX10 8BD Wallingford, Oxon
**Country:** United Kingdom
**Phone:** +1491828557

04-AUG-2005

**Type:** lead organisation
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
**Street:** P.O. Box 2668 - West Lathrop Avenue
**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
**Street:** Avenue E. van Nieuwenhuyse 4
**Town:** B-1160 Brussels
**Country:** Belgium

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
**Contact Person:** Dr. Konrad Gamon **Date:**
**Street:** HenkelstraBe 67
**Town:** D-40551 Düsseldorf
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
**Street:** 33-8, Shiba 5-Chome, Minato-ku
**Town:** 108-0014 Tokyo
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
**Street:** Bingomachi Nomura Building, 1-8, 2-Chome, Bingo-Machi, Chuo-Ku
**Town:** 541-0051 Osaka
**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Oleon N.V.
**Contact Person:** Mr. Filip Bincquet **Date:**
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**Town:** 2520 Oelegem
**Country:** Belgium

**Remark:** Consortium member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
**Street:** 5171 Glenwood Avenue - Suite 402
**Town:** 27612 Raleigh, NC
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
**Contact Person:** Dr. Hans Certa **Date:**
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**Town:** D-45764 Marl
**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
**Street:** Via Medici del Vascello 26
**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc
**Contact Person:** Dr. David Penney **Date:**
**Street:** 900 Threadneedle
**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** United Kingdom

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C12-14 alcohols, CAS 80206-82-2 are 100% linear.

The substance comprises >95% C12, 14 and 16. Components of even chain length, in the range C6-C18 are present.

Commercial products marketed under this CAS number fall into two types with different compositional characteristics. These could have quite different properties, and so it is important to distinguish them, for the scientific interpretation of the data set. These are referred to in this dossier and in the SIAR as Type A and Type B.

Type A products are 100% linear. The substance comprises >90% C12 and 14 (C12>14), <10% C16. Components of even chain length, in the range C6-C18 are present.

Type B products are 100% linear. The substance comprises >95% C12 and 14 (C12<14). Components of even chain length, in the range C8-C18 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C12-14 (CA INDEX NAME)
Fine Oxocol 1213
Kalcohl 6-24
Kalcohl 724A
Lorol 5
Lorol DD
Lorol S
Marlanol 24
Nafol 1214
Sipol C12-C14

Tensioactiv CL 9
Alfol 1214
Alfol 1412
C12-14 alcohols
CO 1270
Dyanol
Epal 12/70
Epal 12/85
Epal 1214
Fatty alcs., C12-14

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C12-14 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.

05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals

for all category members.
Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (5) (21) (27)

### 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

### 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

### 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

### 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

### 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

**Use category:** 9 Cleaning/washing agents and additives
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

19-SEP-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

### 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification NWG or 1 ID No. 1482 and 656.
05-AUG-2005 (29)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C12-14 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.
04-AUG-2005

### 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.
04-AUG-2005

## 2.1 Melting Point

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** solidification point: 17 - 23 degr. C
**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified. Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005 (23)

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
06-JAN-2005 (2)

## 2.2 Boiling Point

**Value:** = 255 - 295 degree C at 1013 hPa

**Method:** other: DIN 51751
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (10)

## 2.3 Density

**Value:** = .82 - .83 at 30 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (19)

**Type:** density

**Value:** = .82 - .83 g/cm³ at 30 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
06-JAN-2005 (10)

**Type:** density
**Value:** = .82 - .83 g/cm³

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Test substance:** It is not possible to determine which compositional Type was tested.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005 (23)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Insufficiently reliable measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for all compositional types of this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
21-OCT-2005 (26)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .0014 - .005 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be

present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.0050 value hPa
Type B: 0.0014 value hPa

**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (2)

## 2.5 Partition Coefficient

**log Pow:** 5.4 - 6 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value. Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
A selection of accepted prediction methods were compared and the results were found to be in good agreement.

**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.

**Flag:** Critical study for SIDS endpoint
22-JUL-2005 (2)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 2.8 - 4.6 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the

SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 4.6 mg/l at a loading rate of 1000 mg/l
Type B: 2.8 mg/l at a loading rate of 1000 mg/l
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (2)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 140 degree C
**Type:** closed cup

**Method:** other: DIN 51785/ISO 2719 (Pensky-Martens)
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
06-JAN-2005 (10)

**Value:** = 140 degree C
**Type:** closed cup

**Method:** other: DIN 51758
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Henkel KGaA Duesseldorf
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is secondary literature and therefore the reliability of the data cannot be verified.Insufficient test substance compositional data were reported for the test results to be reliably assigned to the CAS number.
06-JAN-2005 (23)

## 2.8 Auto Flammability

-

## 2.9 Flammability

**Result:** non flammable

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (19)

## 2.10 Explosive Properties

**Result:** not explosive

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
05-OCT-2005 (19)

## 2.11 Oxidizing Properties

**Result:** no oxidizing properties

**Test substance:** as prescribed by 1.1 - 1.4

**Reliability:** (4) not assignable
11-OCT-2005 (19)

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (4)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:** Type A:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 307000 |
| TGD Non-hydrophobics method: | Koc = 6420 - 30100 |
| TGD Alcohols method: | Koc = 390 - 1240 |
| SRC PCKOCWIN method: | Koc = 330 - 3790 |

Type B:

| | |
|---|---|
| TGD Hydrophobics method: | Koc = 27600 - 96500 |
| TGD Non-hydrophobics method: | Koc = 6420 - 14300 |
| TGD Alcohols method: | Koc = 390 - 710 |
| SRC PCKOCWIN method: | Koc = 330 - 1110 |

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (4)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent from domestic sewage treatment plant (appr. 1000 - 100000 cells/ml)
**Contact time:** 28 day(s)
**Degradation:** = 79 - 97 % after 28 day(s)
**Result:** readily biodegradable
**Kinetic:**

| | |
|---|---|
| 2 day(s) | = 11 - 17 % |
| 11 day(s) | = 14 - 74 % |
| 14 day(s) | = 69 - 85 % |
| 21 day(s) | = 75 - 91 % |
| 28 day(s) | = 79 - 97 % |

**Control Subst.:** other: Sodium acetate

**Method:** other: ISO 10708 (BODIS)
**Year:** 1997
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4
**Method:** BOD-test for Insoluble Substances (BODIS); ISO 10708 (1997) Water quality - Evaluation in an aqueous medium of the ultimate aerobic biodegradability of organic compounds - Determination of biochemical oxygen demand in a two-phase closed bottle test
The test method used is based on OECD test method 301D and the RDA-Blok-Test. Mineral medium was inoculated with activated sludge and stabilized for one week at 18-22 C with continuous stirring. After stabilisation, 200 ml of test medium was filled into 300 ml bottles, aerated until O2 saturation was reached and spiked with test substance by directly weighing into the test vessels. Vessels were filled 2/3, stoppered and shaken continuously at 18-22 C. Degradation was followed by weekly measurements of BOD using an O2-electrode. Oxygen consumption resulting from biodegradation of the test substance was corrected by oxygen uptake of blank inoculum. Degradation rate was calculated as % BOD/ThOD.
**Remark:** The following validity criteria were fulfilled (1) the reference substance reached the pass level of 60% within 14 days, (2) Parallel assays did not differ by greater than 20%, (3) Residual concentration of O2 in test bottles did not fall below 0.5 mg/l, (4) O2 consumption in the blanks was less than 1.5 mg/l.
**Result:** Kinetic of control substance: 2 days = 28 - 33%
7 days = 76 - 73%
14 days = 82 - 80%
21 days = 84 -84%
28 days = 87 - 86%
Two concentrations of effluent were tested: 5 ml/l and 50 ml/l. In the results section, the first value cited is for the 5 ml/l concentration and the second set refers to the 50 ml/l concentration.The test substance degraded >60% over the test period, meeting the 10 day window criterion, therefore it is considered readily biodegradable..
**Test condition:** Test concentration: 100 mg/l related to ThOD (Theoretical Oxygen Demand)
Concentration of effluent: 5 ml/l and 50 ml/l
Test volume: 200 ml
Temperature: 18-22 C
pH: no data
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
28-SEP-2005 (15)

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

This conclusion applies to all compositional Types.

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

30-DEC-2005 (4)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 7200 - 45300

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.
The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Result:** Type A: BCF predicted to be 7200 - 45300
Type B: BCF predicted to be 7200 - 33900

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (4)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Leuciscus idus (Fish, fresh water)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC0:** = 3000
**LC50:** > 5000
**LC100:** > 10000
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on fish-fish test (L15). Test method corresponds to OECD Guideline 203.
**Remark:** This information is from a 1 page summary of the full report but an OECD standard method was used. 10 fish per concentration. Mortalities are recorded at least at 24 hour intervals. The study was carried out prior to 1999. The solubility of lowest carbon chain length in the compound is 3 mg/l, therefore the LC50 is not achieved at the solubility limit.
**Result:** RESULTS: EXPOSED
LC0 = 3000 mg/l
LC50 > 5000 mg/l
LC100 > 10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source:** Henkel KGaA 1999m.
**Test substance:** The test substance corresponds to C12-C14 alcohol, CAS # 80206-82-2. It is not possible to establish the compositional Type of the test substance.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (17)

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = .48 - .77 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give

the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Remark:** The range reflects variable compositional between different commercial products on the market, described validly by the present CAS number.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.43 mg/l
Type B: 0.77 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

30-DEC-2005 (3)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EL50 :** = 63
**Limit Test:** no

**Method:** other: EU guideline 92/69/EWG
**Year:** 1998
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Nominal test concentrations were 1, 3, 10, 30, and 100 mg/L. No solvent was used. Instead, the water accommodated fraction (WAF) was used in the test chambers. Measured concentrations in samples collected from the 10 and 100 mg/L chambers were less than 1% of nominal.
The solubility of the lowest carbon chain length in this compound, C12, is 3 mg/l, therefore the EL50 greatly exceeded the solubility limit.

**Result:** RESULTS: EXPOSED
EL0 30 mg/l
EL50 63 mg/l
EL100 >100 mg/l
Based on nominal loading rates
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Kirch 1998b

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: BioInternational B.V., NJ Horn, NL
Age: 6-24 hours old
Feeding: Green algae 6hours prior to testing
Pretreatment: M4 medium / 20oC / 16h light - 8h dark
Feeding during test: No feeding according to EU guideline
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions

Vehicle, solvent: Not reported
DILUTION WATER
Source: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0, 1, 3, 10, 30, and 100 mg/l
Exposure vessel type: 100 ml flasks
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20.8-20.9 C
Dissolved oxygen: 98.8%
pH mean: 7.9
Intensity of irradiation: approx. 900 lux
Photoperiod: 16 hours light/ 8 hours darkness
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Yes (fluid chromatography of dichloromethane extract)
Measured concentrations of C12-FA and C14-FA were between 0.003 and 0.011 mg/l at 48 hours for 10 and 100 mg/l dose groups.

**Test substance:** This result was measured for a commercial product of compositional Type A.

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (20)

**Unit:** mg/l **Analytical monitoring:** no

**EC50:** = .28 - .23 calculated

**Method:** other

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Result:** The range of results given above reflects variable composition between different commercial products on the market, described by the present CAS number.

The values obtained by prediction are:
Type A: 0.28 mg/l
Type B: 0.23 mg/l

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

11-OCT-2005 (7)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** other algae: Raphidocelis subcapitata
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = .003
**ErL50 :** = .1 - .3
**EbL50 :** = .03 - .3
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 1984
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of LOROL SPEZIAL to R. subcapitata was determined in sealed 72 h growth inhibition toxicity tests. Algal inocula were exposed to test solutions which were not renewed during the test. The tests were repeated three times. The test material was directly added to the WAF preparation vessels using ethanol as a carrier (0.1 mL/L). The vessels were then stirred at approximately 100 rpm for a period of approximately 24 hours, before running off the WAFs for use as the test media.

**Result:** RESULTS: EXPOSED
EbL50 = 0.03 - 0.3 mg/l
ErL50 = 0.1 - 0.3 mg/l
Based on loading rates
For LOROL SPEZIAL, the ranges for the EbL50 and ErL50 were 0.1 to 0.3 mg/L respectively with one exception; the EbL50 in Test 3 was in the range 0.03 to 0.1 mg/L.

**Source:** Palmer and Cann 2000b.

**Test condition:** TEST ORGANISMS
Strain: Raphidocelis subcapitata
Supplier: Institute of Freshwater Ecology, Windermere
Pretreatment: Not reported
Controls: 2 sets of controls (6 replicates and 1 blank flask), one set containing ethanol at 0.1 ml/L
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test medium: Water accommodated fractions
Vehicle, solvent: Ethanol
Concentration of vehicle, solvent: 0.1 ml/l
STABILITY OF TEST CHEMICAL SOLUTIONS:
Considered stable
DILUTION WATER
Source: Not reported
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Loading rates: 0.003, 0.01, 0.03, 0.1, 0.3, and 1 mg/l
Renewal of test solution: None
Exposure vessel type: 287 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 5000 cells/ml
Test temperature: 21.8-24.2
Dissolved oxygen: Not reported

pH mean: 7.3-9.4
Adjustment of pH: None
Intensity of irradiation: Not reported
Photoperiod: Under constant illumination
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: At the start and end of the test. Concentrations of Lorol Spezial in test media decreased by 33-100% over the course of the 72 hour test period.

**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
11-OCT-2005 (22)

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
21-DEC-2005 (7)

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EbL0 :** = .3
**EbL50 :** = 1.2
**ErL50 :** = 1.9
**Limit Test:** no

**Method:** other: EU Commission Directive 92/69/EEC of July 31, 1992 corresponding to OECD-Guideline 201
**Year:** 1999
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The aquatic toxicity was determined in water accommodated fractions. The reported values represent the ErC50 (related to growth rate) and the EbC50 (related to biomass growth).
**Source:** Henkel KGaA 1999l.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but showing greater toxicity are available
11-OCT-2005 (16)

**Species:** other algae: Pseudokirchneriella subcapitata
**Endpoint:** growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEL :** = .6 - 1.2
**ErL50 :** = 2.9
**EbL50 :** = 1.4
**Limit Test:** no

**Method:** OECD Guide-line 201 "Algae, Growth Inhibition Test"
**Year:** 2003
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** WAFs were prepared by loading test medium with the respective amount of the test item. After stirring the contents were left to settle for 24h. The WAFs were filtered prior to use through a non polar filter (0.2 um Millex FG, 50 mm, Millipore).
**Result:** RESULTS: EXPOSED
Growth rate
NOEL = 1.2 mg/l
LOEL = 2.4 mg/l
ErL10 = 0.6 mg/l
ErL50 = 2.9 mg/l
Biomass
NOEL = 0.6 mg/l
LOEL = 1.2 mg/l
EbL10 = 0.8 mg/l
EbL50 = 1.4 mg/l
Based on loading rates
**Source:** Wenzel 2003.
**Test substance:** This result was measured for a commercial product of compositional Type A.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and showing greater toxicity are available
17-OCT-2005 (30)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Type:** aquatic

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** > 10000

**Method:** other: Pseudomonas-Atmungs-Hemmtest, DIN 38412 Teil 27, in Vorbereitung, "Bestimmung der Hemmwirkung von Abwasser auf die Sauerstoffzehrung von Pseudomonas putida."
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** 10000 mg/l was highest concentration tested.
**Source:** Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
**Test condition:** Test substance was directly weighed into test vessel.
**Reliability:** (4) not assignable
not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original report has not been reviewed further because it was not available for review, due to change of business circumstances.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4.
06-AUG-2005 (11)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:**
**EC0:** 10000

**Method:** other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Method conforms with OECD Guide-line 209
**Remark:** LC0/EC0 entspricht der höchsten Prüfkonzentration
Related to: Test substance
**Source:** Henkel KGaA Duesseldorf
Sidobre Sinnova Meaux
**Test substance:** Active Matter = 100 %
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original report has not been reviewed further because it was not available for review, due to change of business circumstances.
Assessment of data quality to current OECD standards is not possible and the study has therefore been assigned Reliability 4.
28-SEP-2005 (12) (13)

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

### 4.7 Biological Effects Monitoring

**Memo:** No data to report
11-SEP-2003

### 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption.

The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (6)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Type:** LD50
**Species:** rat
**Strain:** Wistar
**Sex:** female
**No. of Animals:** 10
**Vehicle:** other: olive oil
**Doses:** 5 & 10 g/kg
**Value:** > 10000 mg/kg bw

**Method:** other: in house procedure
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: No deaths during the study.

CLINICAL SIGNS: No signs of intoxiciation.

NECROPSY FINDINGS: Necropsy not carried out.

POTENTIAL TARGET ORGANS: No indication given.

SEX-SPECIFIC DIFFERENCES: Only females tested.

**Source:** Henkel 1980a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: not reported
- Weight at study initiation: mean weight 190g
- Group size: 10 F
- Controls: no

ADMINISTRATION: Gavage
- Doses: 5 and 10g/kg
- Doses per time period: Single
- Volume administered or concentration: 20 ml/kg constant dose as a solution in olive oil
- Post dose observation period: 14 days

EXAMINATIONS: The animals were observed for mortality and clinical signs.

**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A

**Conclusion:** The rat oral LD50 for this C12-14 alcohol Lorol Spezial type 70 was >10 g/kg. There were no signs of intoxication.

This study is reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14) (18)

**Remark:** Unpublished data ex Henkel KGaA Archive TBD 730111 (12.11.1973)

Mouse oral LD50 >10,000 mg/kg. No mortality and no clinical observations of toxicity. No further data available.
**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
25-JUL-2005 (18)

## 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C8 (1-octanol), C10 (1-decanol), C12 (1-dodecanol), C12-16 (types B&C), C14 (tetradecanol), C16-18 and C16 (hexadecanol) alcohols in support of the statement that C12-14 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (24) (28)

## 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20) including data for C12 (1-dodecanol), C14 (1-tetradecanol), C16 (1-hexadecanol) and C12-16 (type A) alcohols, which support the statement that C12-14 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (24) (28)

## 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London

Hayes Consultancy Service Bromley, Kent
07-MAR-2000

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Occlusive
**Exposure Time:** 24 hour(s)
**No. of Animals:** 6
**Vehicle:** other: none
**PDII:** 3.6
**Result:** moderately irritating
**EC classificat.:** irritating

**Method:** other
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE 24+48+72 hour mean
- Erythema: Individual 1.7, 2.3, 2.0, 1.7, 2.0, 2.3 Group mean 2.0
- Oedema: 1.0 ,1.0 ,1.0 , 1.7, 1.7, 2.0 Group mean 1.4
PII at 24 hours 3.6.

REVERSIBILITY: All scores were 0 by day 6, the study was terminated at day 8.

OTHER EFFECTS: None reported

**Source:** Henkel, 1980a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Male
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: No

ADMINISTRATION/EXPOSURE 24 hour occluded exposure
- Preparation of test substance: Undiluted
- Area of exposure: Not reported.
- Occlusion: Under plaster.
- Vehicle: None
- Total volume applied: 0.5 ml
- Postexposure period: 14 days
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24, 48 and 72 hours and 4, 5, 6, 7 and 8 days after exposure.

**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A
**Conclusion:** Lorol spezial 70 is a skin irritant according to EU criteria based on a group 24+48+72 hour mean score for erythema of 2.

According to GHS criteria the test substance is mild irritant (class 3) with all individual 24+48=72 hour erythema scores between 1.7 - 2.3 (only 2/6 gave a reading of 2.3) following a 24 hour occluded application to rabbit skin.

This study is also reported in Iuclid 2000.

**Reliability:** (2) valid with restrictions
Comparable to guideline study with acceptable restrictions.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14) (18)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Open
**No. of Animals:** 6
**Result:** irritating

**Method:** other: Burckhardt, 1970
**Year:** 1970
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** Erythema was evident at 30 minutes and the degree of irritation increased to 48 hours. After 72 hours the sin was cracked and hard with sloughing between days 9 and 14. Based on a Draize type point score irritation at 24 hours would be considered moderate but severe at 48 hours.

This study was reported in Iuclid 2000.

**Source:** Henkel, 1980a
**Test condition:** This test involved repeated application of 2-3 drops of undiluted test material for 30 seconds for a total of 60 applications. The time of skin contact was 30 minutes.
**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A
**Reliability:** (3) invalid
This is not a currently acceptable regulatory method of assessing skin irritation.

25-JUL-2005 (14) (18)

**Result:** 100% and 50% non-irritant after 24 hours, slightly irritating at 96 hours (after 8 aplications). The degree of irritation increased to 96 hours but there is no information on reversibility.

25% and 10% (20 applications) not irritant up to 10 days although slight effects were seen between days 3 and 6.

The concentration limit for no effect on the skin is 10%.

This study is reported in Iuclid 2000.

**Source:** Henkel, 1980a
**Test condition:** The effect of repeated application to the skin of hairless mice was investigated using different concentrations of the test substance in olive oil. Groups of 5 mice were used.

2-3 drops of the test material or a dilution were applied to the dorsal skin as follows:

100% and 50% twice daily for 4 days (8 applications)
25% and 10% twice daily for 10 days (20 applications)
**Test substance:** TS as prescribed by 1.1 - 1.4
Tradename Lorol Spezial type 70 C12-14 alcohols Type A
**Reliability:** (2) valid with restrictions
Study reasonably well documented, not an accepted method but gives some indication of the effect of repeated exposure to various concentrations of the test material.
25-OCT-2005 (14) (18)

**Species:** human
**Concentration:** undiluted
**Exposure:** Semiocclusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 20
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: patch test based on OECD 404
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test).
**Test condition:** The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.

Study was performed under Good Clinical Practice (GCP).
**Test substance:** Tradename Lorol Spezial C12-14 alcohols Type A
**Conclusion:** Lorol spezial is not irritating to human skin following a 4 hour semi-occlusive exposure.
**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.
**Flag:** Critical study for SIDS endpoint
25-OCT-2005 (9)

**Species:** human
**Concentration:** undiluted
**Exposure:** Open
**Exposure Time:** 1 hour(s)
**No. of Animals:** 20
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** other: open epicutaneous test according to Burckhardt
**Year:** 1996
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No irritating effects or subjective sensations were observed.
**Test condition:** The effect on human skin was investigated:
Undiluted test substance was applied to the forearm with a glass rod for a total application period of 60 minutes. Every

30 seconds, the test substance was gently swabbed with tissue and new test substance applied. Objective findings (erythema, edema) and subjective sensations (e.g. itching, cauterization etc.) were recorded after 15, 30, 45 and 60 minutes.
20 male and female volunteers of average age 35.3 years were tested.

Study was performed under Good Clinical Practice (GCP).

**Test substance:** Tradename Lorol Spezial C12-14 alcohols Type A

**Conclusion:** Lorol spezial was not irritating to human skin following repeated application to non-occluded skin over a period of 1 hour.

**Reliability:** (1) valid without restriction
Test procedure in accordance with generally accepted scientific standards and described in sufficient detail.

25-OCT-2005 (8)

**Result:** No irritation was observed following application to the human skin of a 10% solution of the test substance in ethanol for 8 or 24 hours (patch test) or following repeated application in the Burhardt test.

This study was reported in Iuclid 2000.

**Source:** Henkel, 1980a

**Test condition:** The effect on human skin was investigated:

Single 8 hour application as a 10% solution in ethanol (patch test). 5 volunteers were tested.

Single 24 hour patch test with 10% solution in ethanol

Burckhardt test, repeated aplication (x60) within 30 minutes of 10% solution in ethanol.

**Test substance:** TS as prescribed by 1.1 - 1.4
Tradename Lorol Spezial type 70 C12-14 alcohols Type A

**Reliability:** (2) valid with restrictions
Study reasonably well documented, gives some indication of the effect of exposure to 10% Lorol 70 Spezial in ethanol.

25-OCT-2005 (14) (18)

## 5.2.2 Eye Irritation

**Species:** rabbit
**Concentration:** undiluted
**Dose:** .1 ml
**Comment:** not rinsed
**No. of Animals:** 6
**Vehicle:** none
**Result:** not irritating
**EC classificat.:** not irritating

**Method:** Draize Test
**Year:** 1980
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** AVERAGE SCORE

Draize scoring up to 24 hours post instillation. There was no involvement of the cornea or iris. Minimal conjunctival redness was noted (score <1) at 2 and 6 hours after instillation. All scores at 24 hours were 0.

REVERSIBILITY: Fully reversible by 24 hours after instillation.

OTHER EFFECTS: None reported.

**Source:** Henkel, 1980a
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: Male
- Source: Not reported
- Age: Not reported
- Weight at study initiation: Not reported
- Number of animals: 6
- Controls: The untreated eye served as a control.

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Vehicle: none
- Postexposure period: 24 hours

EXAMINATIONS
- Ophthalmoscopic examination: Not reported.
- Scoring system: Draize
- Observation period: 24 hours
- Tool used to assess score: Not reported.

**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A

**Conclusion:** This C12-14 alcohol is not irritating to the eye when applied undiluted.

**Reliability:** (2) valid with restrictions
Documentation reasonable, observation period short (24 hours) but effects had regressed by this time period so considered valid.

**Flag:** Critical study for SIDS endpoint

25-JUL-2005 (14)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Henkel KGaA TBD790271 (596)

Described as a Draize test the degree of eye irritancy is reported as slight. No further details available.

**Test substance:** C12-14 alcohols Type A

**Reliability:** (4) not assignable
Secondary reference to unpublished data.

25-JUL-2005 (18)

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Unpublished data ex Procter & Gamble Co. Test articles J0171.01 and J0172.02 Rabbit eye irritation, 191-566 (1980) Lit 9925

Reported as a Draize test. Result slightly irritating, no further details available.
**Test substance:** Tradename Lorol Spezial type 70 C12-14 alcohols Type A
**Reliability:** (4) not assignable
Secondary reference to unpublished data.
25-JUL-2005 (18)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C6 (hexanol), C14 (tetradecanol), C16 (hexadecanol) and C18 (octadecanol) which support the conclusion that C12-14 alcohols are not expected to be skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
05-DEC-2005 (24) (25) (28)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C12-14 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), 1-hexadecanol and C18 (octadecanol). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.
14-SEP-2005 (24) (25) (28)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C12-14 alcohols are available from studies of reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, tetradecanol, hexadecanol and octadecanol [Ames].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vitro.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
14-SEP-2005 (24) (25) (28)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol, dodecanol, C12-16 (types A & B), C12-18 (type B), tetradecanol, hexadecanol and octadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be genotoxic in vivo.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
14-SEP-2005 (24) (25) (28)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based

on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C12-14 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14-16 (type A), C16 (hexanol) and data from supporting substances 1-hexanol-2-ethyl, isoamyl alcohol and C12 (octadecanol).

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (1) (24) (25) (28)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C12-14 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (24) (25) (28)

## 5.8.3 Toxicity to Reproduction, Other Studies

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## 5.9 Specific Investigations

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## 5.10 Exposure Experience

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## 5.11 Additional Remarks

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(2) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(4) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

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(12) Henkel KGaA, unpublished data, File 427/1

(13) Henkel KGaA, unpublished data, Final Report 0

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Product safety/Ecology: Unpublished results; Report No. R 9901685.

(17) Henkel KGaA. 1999m. C12-14: Acute toxicity: Fish. Biological research and Product Safety/Ecology: Unpublished results; test substance registration No. 6801.

(18) Iuclid 2000 European Commission - European Chemicals Bureau Alcohols C12-14 Cas# 80206-82-2.

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(25) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

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(29) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 85566-12-7 |
| **CAS No.** | 85566-12-7 |
| **EINECS Name** | Alcohols, C8-10 |
| **EC No.** | 287-621-2 |
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 10-MAY-2006 |
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| **Date of last Update:** | **29-DEC-2005** |
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| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

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20-DEC-2005

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**Remark:** Consortium Member
20-DEC-2005

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**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA.
04-AUG-2005

## 1.0.3 Identity of Recipients

**Remark:** Not required
11-AUG-2003

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C8-10 alcohols, CAS 85566-12-7 are 100% linear.

The substance comprises > 80% C8 and 10, C6<=5%, C12<10%. Components of even chain length, in the range C6-C12 are present.

05-AUG-2005

## 1.1.2 Spectra

**Remark:** Not required
11-AUG-2003

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C8-10 (CA INDEX NAME)
Alfol 810
C8-10 alcs.
CO 1055
Emtrol 1630B
Epal 810
Lincol 810
Lorol C 8-10
Sprout-Off

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C8-10 alcohols.

Composition is described in section 1.1.1, General Substance

Information.
05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 7000 tonnes, consumption 13 000 tonnes (alcohols in range C6-11) - This is publicly-available CEH data for Japan, for 2001.
21-DEC-2005 (16)

## 1.6.1 Labelling

**Remark:** Not required
11-AUG-2003

## 1.6.2 Classification

**Remark:** Not required
11-AUG-2003

## 1.6.3 Packaging

**Memo:** Not required
11-AUG-2003

## 1.7 Use Pattern

**Remark:** Not required
11-AUG-2003

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).
21-DEC-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.
21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Remark:** Not required
11-AUG-2003

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 165 and 71.
05-AUG-2005 (18)

### 1.8.4 Major Accident Hazards

**Remark:** Not required
11-AUG-2003

### 1.8.5 Air Pollution

**Remark:** Not required
11-AUG-2003

### 1.8.6 Listings e.g. Chemical Inventories

**Remark:** Not required
11-AUG-2003

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C8-10 alcohols. There could also be exposure from private use (for consumer products).
05-AUG-2005

### 1.11 Additional Remarks

**Memo:** Not required
11-AUG-2003

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Memo:** Not required

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.
06-JAN-2005 (1)

## 2.2 Boiling Point

**Value:** = 190 - 260 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (12)

## 2.3 Density

**Type:** density
**Value:** = .825 g/cm³ at 20 degree C

**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM. The original reference is not stated and therefore the reliability of the data cannot be verified.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (12)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .089 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be

present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.

**Reliability:** (2) valid with restrictions
Valid with restrictions. The value was predicted using a partial vapour pressure contribution method, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

09-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 3.2 - 4.6 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.

**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.

**Flag:** Critical study for SIDS endpoint

06-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 202 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.

**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

**Result:** The water solubility is estimated to be 202 mg/l at a loading

rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

**Value:** ca. 95 degree C
**Type:** closed cup

**Method:** other: ISO 2719 (Pensky-Martens)
**Test substance:** as prescribed by 1.1 - 1.4

**Source:** Sidobre Sinnova Meaux
**Reliability:** (4) not assignable
This information was obtained from the public IUCLID 2000 CD-ROM
06-JAN-2005 (12)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.

**Result:**
TGD Hydrophobics method: Koc = 56 - 27600
TGD Non-hydrophobics method: Koc = 460 - 2490
TGD Alcohols method: Koc = 54 - 190
SRC PCKOCWIN method: Koc = 28 - 96

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS

dossiers for relevant substances (listed in section 1.0.4 of this Dossier).
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 90 - 1500

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.
**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.
29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** other: Salmo gairdneri (rainbow trout) and Lepomis macrochirus (bluegill)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 2.8 - 5.6
**LC50:** = 6.5 - 10
**Limit Test:** no

**Method:** other: USEPA 1975
**Year:** 1975
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** RESULTS: EXPOSED
NOEC = 5.60 mg/l (Bluegill)
NOEC = 2.80 mg/l (Rainbow trout)
LC50 = 9.96 mg/l (Bluegill)
LC50 = >6.50 <10.0 mg/l (Rainbow trout)
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
The highest concentrations at which there was no discernible effect during the 96-hr bioassay utilizing Alfol 810 was 5.60 mg/l for the bluegill, and 2.80 mg/l for the rainbow trout. The mortality syndrome among fish from those concentrations where mortality was observed was similar. Fish generally became dark and lethargic, lost equilibrium, and expired. The rainbow trout exhibited dark coloration at all concentrations of Alfol 810 greater than 2.80 mg/l.
**Source:** E.G.& G. Bionomics 1975.
**Test condition:** TEST ORGANISMS
Strain: Lepomis macrochirus (Bluegill) and Salmo gairdneri (Rainbow trout)
Supplier: Bluegill obtained from a commercial hatchery in Nebraska, Rainbow trout from a commercial hatchery in Massachusetts
Weight: 1.0 g (Bluegill) and 1.2 g (Rainbow trout)
Feeding: not reported
Pretreatment: Test animals held in laboratory hatchery for at least 30 days prior to test. Fish then acclimated over a 48 hour period prior to testing to test conditions of temperature and water quality.
Feeding during test: none
Control group: 1 control group and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle/solvent: acetone
Concentration of vehicle/solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: not reported
Aeration: none
Alkalinity: not reported
Hardness: 35 ppm CaCO3

Conductance: not reported
TEST SYSTEM
Concentrations: 2.8, 4.2, 6.5, 10, 14, 18, 24 and 37 mg/l for Rainbow trout
4.2, 5.6, 7.5, 10 and 18 mg/l for Bluegill
Renewal of test solution: none
Exposure vessel type: 19.6 liter glass vessels
Number of replicates: 1
Fish per replicate: 10
Test temperature: 21 C for Bluegill and 12 C for Rainbow trout
Dissolved oxygen: 8.9 - 4.2 mg/l
pH mean: 7.1
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: mortality
SAMPLING: 24, 48 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Test substance:** Mixture of Octanol (111-87-5) and Decanol (112-30-1). Composition is comparable with CAS 85566-12-7.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

17-OCT-2005 (6)

**Unit:** mg/l **Analytical monitoring:**

**LC50:** = 2.8 calculated

**Method:** other

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

05-OCT-2005 (7)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no

**EC100:** = 3 calculated

**Method:** other

**Year:** 2005

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. 1 - 10

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.

**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

### 4.6.2 Toxicity to Terrestrial Plants

-

### 4.6.3 Toxicity to Soil Dwelling Organisms

-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

**Memo:** No data to report

11-SEP-2003

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the

oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates.
Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present.
First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles.
Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Source:** de Wolf and Parkerton 1999.

**Reliability:** (2) valid with restrictions

30-OCT-2003 (5)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | Wistar |
| **Sex:** | male |
| **No. of Animals:** | 10 |
| **Vehicle:** | other: olive oil |
| **Doses:** | 5 g/kg |
| **Value:** | > 5000 mg/kg bw |
| **Method:** | other |
| **Year:** | 1979 |
| **GLP:** | no data |
| **Test substance:** | as prescribed by 1.1 - 1.4 |
| **Result:** | MORTALITY: There were no deaths<br><br>CLINICAL SIGNS: There were no signs of toxicity.<br><br>POTENTIAL TARGET ORGANS: No conclusion could be drawn as there were no signs of toxicity and no pathological examination.<br><br>SEX-SPECIFIC DIFFERENCES: Males only tested. |
| **Source:** | Potokar, 1979<br>Hayes Consultancy Service Bromley, Kent |
| **Test condition:** | TEST ORGANISMS:<br>- Source: No data<br>- Age: adult<br>- Weight at study initiation: mean weight 170 g<br>- Controls: No<br><br>ADMINISTRATION:<br>- Doses: 5 g/kg<br>- Doses per time period: single dose<br>- Volume administered or concentration: 1ml/100g in olive oil.<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Clinical signs and mortality. |
| **Test substance:** | Tradename Lorol 810 |
| **Conclusion:** | The rat oral LD50 for Lorol 810 is >5 g/kg. There were no signs of intoxication and no remarkable findings following gross necropsy. |
| | Cited in Iuclid 2000 |
| **Reliability:** | (2) valid with restrictions<br>Study well documented, meets generally accepted scientific principles, acceptable for assessment. |
| **Flag:** | Critical study for SIDS endpoint |

04-AUG-2005 (9) (10)

**Type:** LD50
**Species:** rat
**Strain:** Sherman
**Sex:** male
**Value:** = 9800 mg/kg bw

**Method:** other: Smyth & Carpenter, 1944 & 1948
**Year:** 1951
**GLP:** no
**Test substance:** other TS: decanol mixed isomers

**Test condition:** Groups of 6 male rats received doses of the test material at 10 fold dose intervals, followed by 2 groups of 10 rats at intermediate doses as appropriate.
**Conclusion:** Rat oral LD50 9,800 mg/kg (7,470-12,860). No further details available. Cited in RTECS 2000 under Cas# 85566-12-7.
**Reliability:** (4) not assignable
Summary data on a number of substances, result valid but reporting limited.
04-AUG-2005 (9) (11) (15)

## 5.1.2 Acute Inhalation Toxicity

**Type:** LC50
**Species:** rat
**Strain:** Wistar
**Sex:** male
**No. of Animals:** 5
**Vehicle:** other: atmosphere generated with 55% ethanol
**Doses:** 10% of test substance in ethanol
**Exposure time:** 2 hour(s)

**Method:** other: in house protocol
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Using exactly the same protocol similar results were obtained with Lorol C10.
**Result:** MORTALITY: None of the animals died.

CLINICAL SIGNS: The rats showed no significant signs of intoxication other than falling asleep.

NECROPSY FINDINGS: Neither gross necrospy nor histopathological examination of the respiratory tract and lungs revealed any treament related effects.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: Males only tested.
**Source:** Potokar 1979
Hayes Consultancy Service Bromley, Kent
**Test substance:** Tradename Lorol 810
**Test condition:** TEST ORGANISMS: Rat (Wistar)
- Source: no data
- Weight at study initiation: average body weight 170 g
- Number of animals: 5 males
- Controls: 5 males receiving vehicle

ADMINISTRATION: inhalation
- Type of exposure: 2 hour exposure
- Concentrations: 10% test material in 55% ethanol, a control received ethanol only. The atmospheric concentration was not monitored.
- Particle size: not reported
- Type or preparation of particles:

EXAMINATIONS: The animals were observed for 14 days, at the end of this period gross necropsies were performed and the lungs and respiratory tract removed for histopathological examination.

**Reliability:** (3) invalid
Insufficient study detail and non-standard atmosphere generation.

04-AUG-2005 (10)

**Type:** LC50
**Species:** rat
**Strain:** Sherman
**Sex:** male
**Exposure time:** 8 hour(s)

**Method:** other: screening
**Year:** 1951
**GLP:** no
**Test substance:** other TS: decanol mixed isomers

**Result:** The 8 hour LC50 of decanol (mixed isomers) is greater than the concentrated vapour concentration. No rats died during this exposure.
**Test condition:** Groups of 6 rats were exposed to the concentrated vapours of decanol (mixed isomers) generated by passing air through a disc bubbler at room temperature for up to 8 hours. There was no measurement of vapour concentration.
**Reliability:** (4) not assignable
Summary data on a number of substances, reporting limited. No measurement of vapour concentration.

29-OCT-2004 (15)

## 5.1.3 Acute Dermal Toxicity

**Type:** LD50
**Species:** rabbit
**Strain:** New Zealand white
**Sex:** male
**No. of Animals:** 6
**Vehicle:** other: undiluted
**Doses:** 1000 mg/kg
**Value:** > 1000 mg/kg bw

**Method:** other: in house protocol
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** MORTALITY: All animals survived the exposure period and 14 day observation period.

CLINICAL SIGNS: Confined to slight irritation of the skin reversible in 7 days. No signs of systemic toxicity.

NECROPSY FINDINGS: Not carried out.

POTENTIAL TARGET ORGANS: None identified other than slight skin irritation.

SEX-SPECIFIC DIFFERENCES: Males only tested.

**Source:** Potokar 1979
Hayes Consultancy Service Bromley, Kent

**Test condition:** TEST ORGANISMS: Rabbit (New Zealand White)
- Source: Not reported
- Weight at study initiation: Not reported
- Group size: 6M
- Controls: No

ADMINISTRATION: 24 hour dermal occluded.
- Area covered: 10cm X 10cm
- Occlusion: gauze attached with plaster covered with plastic foil and then with elastic bandage.
- Vehicle: undiluted
- Doses: 1000 mg/kg
- Removal of test substance: Not reported.

EXAMINATIONS: 14 day observation period for mortality, signs of intoxication and local skin reaction.

**Test substance:** Tradename Lorol 810

**Conclusion:** The rabbit dermal LD50 for Lorol 810 is >1000 mg/kg (24 hour occluded exposure). There were no signs of systemic toxicity only slight reversible skin irritation.

Cited in Iuclid 2000

**Reliability:** (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag:** Critical study for SIDS endpoint

04-AUG-2005 (9) (10)

**Type:** LD50
**Species:** rabbit
**Vehicle:** other: undiluted
**Value:** = 3560 ml/kg bw

**Method:** other
**Year:** 1951
**GLP:** no
**Test substance:** other TS: decanol (mixed isomers)

**Result:** Rabbit dermal LD50 3.56 ml/kg (2.5-5.76). Vale cited in RTECS 2004.

**Test condition:** The undiluted material was applied to the skin of rabbit under a rubber dam and the animals observed for 14 days.

**Reliability:** (4) not assignable
Summary data on a number of substances, result probably valid but reporting limited.

29-OCT-2004 (11) (15)

### 5.1.4 Acute Toxicity, other Routes

**Remark:** Not required OECD or HPV endpoint.
**Source:** The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent
07-MAR-2000

### 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Species:** rabbit
**Concentration:** 100 %
**Exposure:** Occlusive
**Exposure Time:** 8 hour(s)
**No. of Animals:** 5
**Vehicle:** other: undiluted
**Result:** slightly irritating
**EC classificat.:** not irritating

**Method:** other:
**Year:** 1979
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Result:** No individual scores are given. The test material is reported as producing slight irritation which is reversible over the 14 day observation period. A score of 2,2 is reported but it is not clear exactly what this refers to.
**Source:** Potokar, 1979
Hayes Consultancy Service Bromley, Kent
**Test condition:** TEST ANIMALS:
- Strain: Albino rabbits
- Sex: Male
- Age: Adult
- Number of animals: 5

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Area of exposure: Not reported
- Occlusion: Yes
- Vehicle: None
- Exposure period: 8 hours
- Postexposure period: 14 days
- Removal of test substance: Not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: immediately after removal of patch then at 24 hours, observed until 14 days.

**Test substance:** Tradename Lorol 810
**Conclusion:** Based on the limited data available it is considered that Lorol 810 is slightly irritating to the skin but unlikely to be a skin irritant under GHS or EU criteria.

Cited in Iuclid 2000.
**Reliability:** (4) not assignable

Limited reporting of results, documentation insufficient for assessment.
**Flag:** Critical study for SIDS endpoint
04-AUG-2005 (9) (10)

**Species:** rabbit
**Concentration:** undiluted
**Exposure:** Open
**Exposure Time:** 24 hour(s)
**No. of Animals:** 5
**Result:** irritating

**Year:** 1951
**GLP:** no
**Test substance:** other TS: mixed isomers of decanol

**Result:** The degree of skin irritancy is grade 5 described as strong erythema, oedema or slight necrosis. Decanol (mixed isomers) is irritant to the skin in this test.
**Test condition:** This is a non-standard test. The test material is applied for a 24 hour uncovered exposure in a volume of 0.01 ml of either the undiluted material or dilutions in water or solvent. For this test the material was applied undiluted. Skin irritation is graded on a 10 point scale (this is described fully in Smyth et al, 1949)
**Reliability:** (3) invalid
Non standard method not comparable to modern guidelines.
29-OCT-2004 (15)

## 5.2.2 Eye Irritation

**Result:** Decanol (mixed isomers) was classified as group 2 (0.5 ml undiluted yields score of >1 but not greater than 5. This may be described as moderately irritating.
**Test condition:** This eye irritation assay involves treating the eye with different volumes and concentrations of the test substance and evaluating the corneal and iritic effects after 18-24 hours before and after fluorescein staining (score maximum 20). A score of 5 is considered to represent severe injury. A 10 point grading scale incorporating the scores at various dilutions and volumes is used to classify the observed effects. Method of Carpenter & Smyth, 1946. This method is not an accepted method for evaluation of eye irritancy and the results cannot be considered as valid.
**Test substance:** Reported as decanol (mixed isomers)
**Reliability:** (3) invalid
Non standard method as described above, not comparable with modern guidelines, not considered valid for classification of irritation.
04-AUG-2005 (15)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C6 (hexanol), C10-16

alcohols and C12 (dodecanol) which support the conclusion that C8-10 alcohols are not expected to be skin sensitisers.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a skin sensitiser.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of sensitisation potential is based are either guideline or similar studies or publications with sufficient detail for assessment.

05-DEC-2005 (13) (17)

## 5.4 Repeated Dose Toxicity

**Remark:** There is a lack of significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A), 1-hexadecanol, C16-18 and C18 unsaturated alcohols, 1-octadecanol (supporting), 1-docosanol and alcohols C24-34 (supporting). The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of systemic toxicity is based are either comparable to guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (13) (14) (17)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C8-10 alcohols are available from studies of reliability 1 or 2 for 1-hexanol [Ames], 1-octanol [Ames], 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion] and 1-dodecanol (supporting) [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vitro is based are either guideline or comparable

studies or publications with sufficient detail for assessment.
12-SEP-2005 (13) (17)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline or similar studies or publications with sufficient detail for assessment.

25-OCT-2005 (8) (13) (14) (17)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproduction screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that C8-10 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols type C, and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of effect on the reproductive potential is based are either comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (8) (17)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C8-10 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for developmental toxicity is based are either guideline or similar studies or publications with sufficient detail for assessment.

12-SEP-2005 (13) (17)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(5) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(6) E.G.& G. Bionomics. 1975. Acute toxicity of two Conoco compounds to bluegill (lepomis macrochirus) and rainbow trout (Salmo gairdneri). Bioassay report submitted to Conoco Chemicals, Ponca City, Oklahoma.

(7) Fisk, P.R et al, 2005: Ecotoxicology: Interpretation of data for multi-component substances; Annex IV to the Long Chain Alcohols SIAR

(8) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

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(16) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(17) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(18) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

**Existing Chemical** ID: 85665-26-5
**CAS No.** 85665-26-5
**EINECS Name** Alcohols, C10-12
**EC No.** 288-117-5

**Producer Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Substance Related Part**
**Company:** Shell Chemicals Ltd.
**Creation date:** 18-JAN-2006

**Memo:** MERGED JAN 2006

**Printing date:** 10-MAY-2006
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**Reliability (profile):** Reliability: without reliability, 1, 2, 3, 4
**Flags (profile):** Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

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23-AUG-2005

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20-DEC-2005

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20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
04-AUG-2005

## 1.0.3 Identity of Recipients

**-**

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members.

In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |

| | |
|---|---|
| Alcohols, C12-13 | 75782-86-4 |
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

-

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as C10-12 alcohols, CAS 85665-26-5 are 100% linear.

The substance comprises >90% C10 and 12, <=5% C14. Components of even chain length, in the range C8-C16 are present.

05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** Some synonyms, including a selection of commercial product names, are:

Alcohols, C10-12 (CA INDEX NAME)
Alc., C10-12
Alcs., C10-12
Alfol 1012
C10-12 alcohols
C10-12 alcs.
C10-12 alkanols
Epal 1012

**Source:** Synonyms listed in various sources in the public domain, including the CAS Registry and Chemfinder website

21-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in C10-12 alcohols.

Composition is described in section 1.1.1, General Substance Information.

05-AUG-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.
21-DEC-2005 (5) (8) (12)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic, textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

## 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

## 1.8.1 Occupational Exposure Limit Values

-

## 1.8.2 Acceptable Residues Levels

-

## 1.8.3 Water Pollution

**Remark:** WGK Classification 1 ID No. 71 and 1482.

05-AUG-2005 (14)

## 1.8.4 Major Accident Hazards

-

## 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

-

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of C10-12 alcohols. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7.

04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of melting point. It is not possible to estimate with confidence what the melting range might be.

21-OCT-2005

## 2.2 Boiling Point

**Value:**

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. This could have a significant influence on the value of boiling point. It is not possible to estimate with confidence what the boiling range might be.

21-OCT-2005

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.

**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (11)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .011 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
09-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 4.6 - 5.4 at 25 degree C

**Method:** other (calculated): based on values of components
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, as prescribed by 1.1 - 1.4. There cannot be a single value of log Kow for this mixture, but the values for the components present are relevant. The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The range of values is based on reliable measured values for the components.
**Flag:** Critical study for SIDS endpoint
06-JAN-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 34 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 34 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (1)

**2.6.2 Surface Tension**

-

**2.7 Flash Point**

-

**2.8 Auto Flammability**

-

**2.9 Flammability**

-

**2.10 Explosive Properties**

-

**2.11 Oxidizing Properties**

-

**2.12 Dissociation Constant**

-

**2.13 Viscosity**

-

**2.14 Additional Remarks**

-

## 3.1.1 Photodegradation

**Remark:** The substance has a range of components, as prescribed by section 1.1-1.4. All components are predicted to be photodegraded with half-lives ranging between ca. 10-30 hours, based on prediction using the SRC AOPWIN v1.91 program, with limited validation.

Branched components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly faster than linear components of equivalent carbon number.

Please refer to the discussions of photdegradation for substances of specific chain length (i.e. essentially pure) for details of predicted/measured rate constants and individual half lives. Refer to the dossiers for the relevant substances (see section 1.0.4 for a list of long chain alcohols CAS).

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Year:** 2005

**Result:** It is not realistic to provide in-depth discussion on the environmental distribution of this substance, which contains a mixture of components, as described in section 1.1-1.4. However, it will be useful to refer to the distribution for substances of specific chain length (i.e. essentially pure). Refer to the dossiers for the relevant substances (see section

1.0.4 for a list of long chain alcohols CAS).
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

### 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. None of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Hydrophobics equation is the most conservative across the category, except at the shortest chain lengths. While this method is not intended for use with alcohols, measured adsorption coefficients in the range C12-18 (van Compernolle et al, in press) suggest that this method is relevant for these substances.

Where available, measured log Kow values were used as inputs into the calculation.
**Remark:** For the components of this substance, the adsorption factors are calculated to be in the range indicated above.
**Result:** TGD Hydrophobics method: Koc = 2500 - 6400
TGD Non-hydrophobic method: Koc = 6330 - 96500
TGD Alcohols method: Koc = 190 - 390
SRC PCKOCWIN method: Koc = 96 - 330

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only at the upper limit of the range
**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.
29-DEC-2005 (3)

### 3.4 Mode of Degradation in Actual Use

-

### 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** The substance has a range of components, As prescribed by section 1.1-1.4. All components are predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 1500 - 7200

**Method:** other: calculated (based on values of components)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.

Where available, measured log Kow values were used as inputs into the calculation.

**Remark:** For the components of this substance, the bioconcentration factors are calculated to be in the range indicated above. Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.

The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value is based on estimates for the components of the substance, made using accepted calculation methods.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** = 2.1 calculated

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** = 1.1 calculated

**Method:** other: calculated (partition model)
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Unit:** mg/l **Analytical monitoring:**
**EC10:** calculated
**EC50:** ca. .1 - 1

**Method:** other: read-across based on grouping of substances (category approach)/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Acute toxicity to algae cannot easily be estimated for multi-component alcohols, but has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels. Specifically, measured and predicted effects in Daphnia and fish for this substance were taken into account, together with interpretation across the Category of the relationship between effect concentrations for these organisms and effect concentrations for algae.

Examination of the available measured data across the long chain alcohols Category suggest that for multi-component substances, algal EC50 values can be estimated based on Daphnia EC50 values, which are the most applicable; although it is possible that effects on algae could be slightly more severe. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by partition modelling rather than measured.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (4)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

-

## 4.6.2 Toxicity to Terrestrial Plants

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## 4.6.3 Toxicity to Soil Dwelling Organisms

-

## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

-

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and

pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (6)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22) including data for C8 (1-octanol), C8-10, C10 (1-decanol) and C12 (1-dodecanol) alcohols, which support the statement that C10-12 alcohols are expected to be of low acute oral toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg
**Reliability:** (2) valid with restrictions
The studies on which the conclusion C10-12 alcohols are expected to be of low toxicity (LD50 >2000 mg/kg) is based are either comparable to guideline studies or publications with sufficient detail for assessment.
12-SEP-2005 (9) (13)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the substantially saturated vapour concentration. This includes data for C8 (1-octanol), C8-10, C10 (1-decanol), C12 (1-dodecanol) and C14 (tetradecanol) alcohols in support of the statement that C10-12 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion that C10-12 alcohols are expected to be of low toxicity with the LC50 expected to be greater than the substantially saturated vapour concentration is based are comparable to guideline studies or publications with sufficient detail for assessment.
12-SEP-2005 (9) (13)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20) including data for C10(1-decanol) and

C12 (1-dodecanol) alcohols, which support the statement that C10-12 alcohols are expected to be of low acute dermal toxicity LD50 >2000 mg/kg. (Refs 2, 3)

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion C10-12 alcohols are expected to be of low toxicity (LD50 >2000 mg/kg) is based are either comparable to guideline studies or publications with sufficient detail for assessment.

12-SEP-2005 (9) (13)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Remark:** The skin irritation potential of alcohols with a chain length C12 and above (e.g. 1-dodecanol) is classified as non-irritant - mild. On the basis that some of the linear alcohols in range C6 - C10 have a skin irritation potential, it cannot be excluded that alcohols containing a significant amount of 1-decanol are without a skin irritation potential. C10-12 alcohol is therefore expected to be a skin irritant.

Data in support of this conclusion are available for C8 (1-octanol), C10 (1-decanol) and C12 (1-dodecanol) alcohols which support the conclusion that C10-12 alcohols are expected to be irritating to the skin.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** C10-12 alcohols are expected to be rritating to the skin.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion that C10-12 alcohols are expected irritating to the skin are based are comparable to guideline studies or publications with sufficient detail for assessment.

29-DEC-2005 (9) (13)

## 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants. This includes data available for C10 (1-decanol) and C12 (dodecanol) which support the conclusion that C10-12 alcohols are expected to be eye irritants.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** C10-12 alcohols are expected to be irritating to the eyes.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion that C10-12 alcohols are expected irritating to the eye is based are guideline and

comparable studies or publications with sufficient detail for assessment.

29-DEC-2005 (9) (13)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18, all assays were negative. Included are negative data from guinea pig maximisation tests for C6 (hexanol), C12 (dodecanol), C14 (tetradecanol) and C16 (hexadecanol) which support the conclusion that C10-12 alcohols are not expected to be skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** C10-12 alcohols are not expected to be skin sensitisers.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion that C10-12 alcohols are not expected to be skin sensitisers are based on guideline and comparable studies or publications with sufficient detail for assessment.

07-JAN-2006 (9) (13)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for C10-12 alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-hexanol, 2-ethyl hexanol (supporting), 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type A) and 1-hexadecanol. The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion that C10-12 alcohols are expected to be of low systemic toxicity following repeated exposure are based are comparable to guideline studies or publications with sufficient detail for assessment.

14-SEP-2005 (9) (13)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may

be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5 to C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for C10-12 alcohols are available from studies of reliability 1 or 2 for 1-hexanol [Ames], 1-octanol [Ames], 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], 1-dodecanol, tetradecanol and hexadecanol (supporting) [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vitro is based are either guideline or comparable studies or publications with sufficient detail for assessment.

25-OCT-2005 (9) (13)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances C5 to C24-34) including data for 1-octanol and 1-decanol, dodecanol, tetradecanol and hexadecanol are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of genotoxic potential in vivo is based are either guideline or similar studies or publications with sufficient detail for assessment.

25-OCT-2005 (7) (9) (10) (13)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially

linear alcohols.

Data in support of the conclusion that C10-12 alcohols are not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to impair fertility.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of effect on the reproductive potential is based are either comparable to guideline studies or publications with sufficient detail for assessment.

13-SEP-2005 (7) (9) (10) (13)

### 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that C10-12 alcohols are not expected to be developmental toxicants in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion for lack of potential for developmental toxicity is based are either comparable to guideline or publications with sufficient detail for assessment.

13-SEP-2005 (9) (10) (13)

### 5.8.3 Toxicity to Reproduction, Other Studies

-

### 5.9 Specific Investigations

-

### 5.10 Exposure Experience

-

### 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(5) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(6) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(7) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(8) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(9) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(10) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(11) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(12) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(13) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

(14) Water hazard class according to the Administrative Regulation on Water Endangering Substances (Verwaltungsvorschrift wassergefährdende Stoffe; VwVwS as of May 17, 1999).

# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 90583-91-8 |
| **CAS No.** | 90583-91-8 |
| **EINECS Name** | Tridecanol, branched and linear |
| **EC No.** | 292-296-5 |
| **Producer Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Substance Related Part** | |
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
| **Revision date:** | |
| **Date of last Update:** | **11-MAY-2006** |
| **Number of Pages:** | **36** |
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** sponsor country
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**Country:** United Kingdom
**Phone:** +1491828557

23-AUG-2005

**Type:** cooperating company
**Name:** Aliphatic Alcohols Consortium, The Soap and Detergent Association
**Contact Person:** Hans Sanderson **Date:**
**Street:** 1500 K Street NW, Suite 300
**Town:** 20005 Washington DC
**Country:** United States

**Remark:** Industry Consortium
23-AUG-2005

**Type:** cooperating company
**Name:** Arizona Chemical Company
**Contact Person:** Ms. Jenifer A. Whittington **Date:**
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**Town:** 31402 Savannah, GA
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** CEFIC
**Contact Person:** Dr. Christophe Sene **Date:**
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**Town:** B-1160 Brussels
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Cognis Deutschland GmbH
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**Country:** Germany

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Kao Corporation
**Contact Person:** Mr. Yutaka Kasai **Date:**
**Street:** 2-1-3 Bunka, Sumida-ku
**Town:** 131-8501 Tokyo

**Country:** Japan

**Remark:** Consortium Member
20-DEC-2005

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**Name:** Mitsubishi Chemical Corporation
**Contact Person:** Dr. Yasukazu Uchida **Date:**
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**Town:** 108-0014 Tokyo
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** New Japan Chemical Co. Ltd.
**Contact Person:** Mr. Kango Fujitani **Date:**
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**Town:** 541-0051 Osaka
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Rhodia Inc.
**Contact Person:** Dr. Glenn Simon **Date:**
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**Town:** 27612 Raleigh, NC
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** SASOL Germany GmbH
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**Town:** D-45764 Marl
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**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol Italy SpA
**Contact Person:** Enrico Dallara **Date:**
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**Town:** 20138 Milano

**Country:** Italy

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Sasol North America Inc.
**Contact Person:** Dr. David Penney **Date:**
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**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
04-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members. In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |

| | |
|---|---|
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** Tridecanol, branched and linear
**Smiles Code:** Not applicable for a mixture
**Mol. Formula:** C13 H28 O1
**Mol. Weight:** 200.37
21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as tridecanol, branched and linear, CAS 90583-91-8 are 5% linear.

The substance comprises >95% C13. Components of odd chain length are present.
05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** There are no Synonyms listed in Chemical Abstracts
06-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in branched and linear tridecanol.

Composition is described in section 1.1.1, General Substance Information
21-SEP-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (6) (9) (13)

## 1.6.1 Labelling

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## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic,

textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

-

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

-

### 1.8.4 Major Accident Hazards

-

### 1.8.5 Air Pollution

-

### 1.8.6 Listings e.g. Chemical Inventories

-

### 1.9.1 Degradation/Transformation Products

-

### 1.9.2 Components

-

### 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of branched and linear tridecanol. There could also be exposure from private use (for consumer products).

05-AUG-2005

### 1.11 Additional Remarks

-

### 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7

04-AUG-2005

### 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Value:** ca. 29 degree C

**Method:** other: (calculated) SRC MPBPVP v1.40
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Validation of melting point prediction using this method shows that the calculated values are close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.2 Boiling Point

**Value:** = 279 degree C

**Method:** other: (calculated) SRC MPBPVP v1.40
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint

21-OCT-2005 (12)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00057 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** Result = 5.7 X 10-4 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 5.56 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .38 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.38 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 19.8837E-12 cm3/molecule.sec
Half-life: 19.4 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Linear components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly more slowly than branched components of equivalent carbon number, but the reported half-life represents a reasonable estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:
Molecular weight 200.4
Data temperature 25 deg C
Log Kow 5.56
Water Solubility 0.38 mg/l
Vapour pressure 0.057 Pa
Melting point 29 deg C
half life in air 19.6 h
half life in water and soil 720 h
RESULTS:
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 1.81% |
| Soil | 95.7% |
| Water | 0.30% |
| Fish | 5.39E-03% |
| Sediment | 2.13% |

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 67.4 | 0.016 | 0.00015 |
| % in water | 1.36 | 8.65 | 0.0117 |
| % in sediment | 14.3 | 91.3 | 0.123 |
| % in soil | 16.9 | 0.0040 | 99.9 |

The results reflect that the ultimate fate of tridecanol, branched and linear, is dependent on its route of release into the environment. Tridecanol, branched and linear released to air would partially precipitate to soil and water. There is relatively little
movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.

In water, the adsorption coefficient of tridecanol, branched and linear results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (4)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category. The measured log Kow value of 5.51 was used in the TGD calculation methods.

**Result:** TGD Hydrophobics method: Koc = 40100
TGD Non-hydrophobics method: Koc = 8150

TGD Alcohols method: Koc = 470
SRC PCKOCWIN method: Koc = 530

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

29-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)
**Year:** 2005
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 10600

**Method:** other: calculated (Veith et al, 1979)
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.The measured log Kow value of 5.51 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

## 4.5.1 Chronic Toxicity to Fish

-

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

## 4.6.1 Toxicity to Sediment Dwelling Organisms

-

## 4.6.2 Toxicity to Terrestrial Plants

-

## 4.6.3 Toxicity to Soil Dwelling Organisms

-

## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

-

## 4.7 Biological Effects Monitoring

-

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (7)

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Oral: Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, data for undecanol and C12-13 alcohols. This data supports the statement that Tridecanol is expected to be of low acute oral toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (14)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C11 (undecanol), C12-16 and tridecanol (Cas 112-70-9) alcohols in support of the statement that Tridecanol branched and linear Cas 90583-91-8 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (14)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, data for undecanol and C12-13 alcohols. This data supports the statement that Tridecanol is expected to be of

low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (14)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. For the subcategory of essentially linear alcohols, of which Tridecanol (branched and linear Cas 90583-91-8) is a member, the skin irritation potential for the higher members in the range C12 - C16 is mild - essentially non-irritant. This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, together with data on C12-13 and C12-16 alcohols. This supports the conclusion that Tridecanol (branched and linear, Cas 90583-91-8) is expected to be mildly irritating to the skin.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Tridecanol (branched and linear) is expected to be mildly irritating to the skin.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
11-MAY-2006 (14)

## 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants while alcohols of chain length >C12 are essentially non-irritating to the eye. Data available for C12-13 and C12-15 alcohols support the conclusion that tridecanol (branched and linear) alcohol is expected to be essentially non-irritating to the eye.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Tridecanol (branched and linear) is expected to be essentially non-irritating to the eye.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (14)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A), C14-16 (type A) and C16 (hexadecanol) alcohols which support the conclusion that Tridecanol (branched and linear) alcohols are not expected to be skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
05-DEC-2005 (14)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for tridecanol (linear and branched) alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type B) and 1-hexadecanol . The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** ected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (10) (14)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for tridecanol (branched and linear) are available from studies of

reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (14)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (8) (10) (11) (14)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that tridecanol (branched

and linear) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14 -16 (type A) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (8) (14)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that tridecanol (branched and linear) is not expected to be a developmental toxicant in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (10) (11) (14)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

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(11) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(12) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(13) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

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# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 90583-91-8 |
| **CAS No.** | 90583-91-8 |
| **EINECS Name** | Tridecanol, branched and linear |
| **EC No.** | 292-296-5 |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Shell Chemicals Ltd. |
| **Creation date:** | 18-JAN-2006 |

| | |
|---|---|
| **Memo:** | MERGED JAN 2006 |
| **Printing date:** | 11-MAY-2006 |
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| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

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**Town:** 77079 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemical Company
**Contact Person:** Ms. Susan O. Antrican **Date:**
**Street:** 910 Louisiana Street, One Shell Plaza
**Town:** 77002 Houston, TX
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

**Type:** cooperating company
**Name:** Shell Chemicals Limited
**Contact Person:** Mr. Gauke Veenstra **Date:**
**Street:** P.O. Box 162
**Town:** NL-2501AN The Hague
**Country:** Netherlands

**Remark:** Consortium member
20-DEC-2005

**Type:** cooperating company
**Name:** The Procter & Gamble Company
**Contact Person:** Dr. Scott E Belanger **Date:**
**Street:** Miami Valley Innovation Center, P.O. Box 538707
**Town:** 45253-8707 Cincinatti, OH
**Country:** United States

**Remark:** Consortium Member
20-DEC-2005

## 1.0.2 Location of Production Site, Importer or Formulator

**Remark:** There are production sites for long chain alcohols in Belgium, Germany, Italy, Japan, UK, and USA
04-AUG-2005

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

**Comment:** This substance is part of a Category of long chain aliphatic alcohols, set up on grounds of structural similarity.

**Remark:** The Long Chain Alcohols Category consists of aliphatic alcohols within a carbon chain length range of C6-C22. The Category covers 30 CAS numbers. The Category members include alcohols with varying compositions and structures. Composition depends on the route to manufacture and the related feedstocks. Most of the alcohols have predominantly linear carbon chains but certain manufacturing processes create branched or unsaturated structures. Commercial products are primarily mixtures of carbon chain lengths.

Many of the Category members are complex reaction products, containing a range of aliphatic alcohol components, of varying carbon chain lengths. There is considerable overlap between the compositions of certain Category members. In some cases, a commercial product could be accurately described by any of several different CAS numbers and names. Indeed, for some commercial products marketed by international companies, different CAS numbers may be used in different parts of the world (usually for historical reasons, including commercial, regulatory or inventory status). Where this is the case, data are filed on one dossier only, for the ‚preferred' CAS number (usually indicated by the company). More detailed information is presented in the confidential annex to the SIAR.

The individual substances covered by the Long Chain Alcohols Category are:

| CHEMICAL NAME | CAS no. |
|---|---|
| 1-Hexanol | 111-27-3 |
| 1-Octanol | 111-87-5 |
| 1-Decanol | 112-30-1 |
| 1-Undecanol | 112-42-5 |
| 1-Tridecanol | 112-70-9 |
| 1-Tetradecanol | 112-72-1 |
| 1-Pentadecanol | 629-76-5 |
| 1-Hexadecanol | 36653-82-4 |
| 9-Octadecen-1-ol, (9Z)- | 143-28-2 |
| 1-Eicosanol | 629-96-9 |
| 1-Docosanol | 661-19-8 |
| Alcohols, C12-15 | 63393-82-8 |
| Alcohols, C9-11 | 66455-17-2 |
| Alcohols, C12-18 | 67762-25-8 |
| Alcohols, C16-18 | 67762-27-0 |
| Alcohols, C14-18 | 67762-30-5 |
| Alcohols, C10-16 | 67762-41-8 |
| Alcohols, C8-18 | 68551-07-5 |
| Alcohols, C16-18 and C18 Unsaturated | 68002-94-8 |
| Alcohols, C14-18 and C16-18-unsatd. | 68155-00-0 |
| Alcohols, C14-16 | 68333-80-2 |
| Alcohols, C6-12 | 68603-15-6 |
| Alcohols, C12-16 | 68855-56-1 |
| Alcohols, C12-13 | 75782-86-4 |

| | |
|---|---|
| Alcohols, C14-15 | 75782-87-5 |
| Alcohols, C12-14 | 80206-82-2 |
| Alcohols, C8-10 | 85566-12-7 |
| Alcohols, C10-12 | 85665-26-5 |
| Tridecanol, branched and linear | 90583-91-8 |
| Alcohols, C18-22 | 97552-91-5 |

These substances are produced by Consortium Members using trade names with numerical codes. These names include

ALCHEM
ALFOL
CO
DOBANOL
EPAL
HYDRENOL
ISALCHEM
KALCOL
LANETTE
LIAL
LINEVOL
LOROL
NACOL
NAFOL
NEODOL
OCENOL
SAFOL
TA

06-OCT-2005

**Comment:** Key studies are flagged in the SIDS dossier. These are studies with the highest reliability/adequacy.

**Remark:** If several studies showed comparable reliability/ adequacy, the study with the lowest LC/LD/EC50 or NOEC/ NOAEL was indicated as the key study. For some endpoints, fully reliable results were not available and it was necessary to use a weight of evidence including results of studies of non-assignable reliability. In such cases the results are identified as key studies as they are of high importance to the data set.

For transparency, some study summaries in the SIDS dossier were transferred from the previously published version of IUCLID. In some cases, it was not possible to retrieve the original literature/study reports using the reported citation or as a result of literature searching. In some cases, change of business ownership meant that internal study reports cited in previous summaries could not be accessed. In some other cases, e.g. certain non-SIDS endpoints, and in areas where a very large amount of literature has been published, it was not considered necessary to pursue all individual published sources due to weight of evidence of more reliable results. In all cases, reliability (4) applies, because the original documentation has not been reviewed in the development of the dossier.

04-AUG-2005

## 1.1.0 Substance Identification

**IUPAC Name:** Tridecanol, branched and linear
**Smiles Code:** Not applicable for a mixture
**Mol. Formula:** C13 H28 O1
**Mol. Weight:** 200.37
21-DEC-2005

## 1.1.1 General Substance Information

**Substance type:** organic
**Physical status:** liquid

**Remark:** The substances in this Category have a range of composition and purity. Some information is confidential. Non-confidential data are summarised here.

Of the commercial products associated with the Consortium members, those identified as tridecanol, branched and linear, CAS 90583-91-8 are 5% linear.

The substance comprises >95% C13. Components of odd chain length are present.
05-AUG-2005

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

**Remark:** There are no Synonyms listed in Chemical Abstracts
06-OCT-2005

## 1.3 Impurities

**Remark:** Some of the substances in the Long Chain Alcohols Category contain other alcohols (e.g. decanol may be present in dodecanol). In the context of the Category, these are considered to be by-products rather than impurities. True impurities, with a chemical structure different from the definition of the Category, are not present in branched and linear tridecanol.

Composition is described in section 1.1.1, General Substance Information
21-SEP-2005

## 1.4 Additives

**Remark:** No additives are used.
05-AUG-2005

## 1.5 Total Quantity

**Quantity:** ca. 1500000 - 3000000 tonnes 2004

**Remark:** The quantity stated above is an estimated global total annual consumption. This figure, and the data below, relate to totals for the entire Long Chain Aliphatic Alcohols HPV Category, including both 'sponsored' Category members and 'supporting' substances (refer to the SIAR).

USA: production + import ca. 650 000 - 2 000 000 tonnes in 2002 (IUR data). Production ca. 620 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Western Europe: consumption ca. 700 000 tonnes in 2004 (APAG/CEFIC data). Production ca. 710 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Japan: production + import total ca. 150 000 tonnes per year (published data). Production ca. 250 000 tonnes (2002 survey of the Consortium member companies). Both figures are totals for all category members.

Commercial production figures for specific CAS, or narrow ranges of chain length, are confidential.

For this substance, more specific data are available in the public domain:

Japan: Production 62 000 tonnes, imports 60 000 tonnes, exports 5 000 tonnes, consumption 117 000 tonnes (alcohols in range C12-18)- This is publicly-available CEH data for Japan, for 2002.

21-DEC-2005 (6) (9) (13)

## 1.6.1 Labelling

-

## 1.6.2 Classification

-

## 1.6.3 Packaging

-

## 1.7 Use Pattern

-

## 1.7.1 Detailed Use Pattern

**Remark:** Across the Long Chain Alcohols Category, approximately 50% of the total production volume is used directly in final products, including paints, lubricants, paper, plastic,

textiles, leather, plaster, formwork oils, household products and personal care/cosmetic products.

The remainder is processed as an intermediate (with approximately 65% of the intermediate volume being site limited).

21-DEC-2005

### 1.7.2 Methods of Manufacture

**Remark:** Aliphatic alcohols are manufactured by a number of processes, but these can be divided into two general categories:

Oleochemical - the feedstocks for the most common oleochemical-based processes include plant or animal based oils or fats: coconut, palm kernel oil and tallow fat, or other triglycerides.

Petrochemical and other synthetic processes - the most commonly used processes use different feedstocks - olefins (alpha and internal), ethylene, propylene oligomers. Some Category members are produced using olefins derived from the Fischer-Tropsch process.

Some commercially available products are blends of two or more specific chain length alcohols to produce mixtures.

Different manufacturing methods can lead to different compositional profiles; further details are given in Annex I to the SIAR.

Compositional information given in chapter 1.1-1.4 represents typical composition. Specific batches may be subject to variation.

21-DEC-2005

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

-

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

-

### 1.8.4 Major Accident Hazards

-

### 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

-

## 1.9.1 Degradation/Transformation Products

-

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Remark:** Exposure could arise in association with production, formulation and industrial use of branched and linear tridecanol. There could also be exposure from private use (for consumer products).

05-AUG-2005

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

**Type of Search:** Internal and External

**Remark:** All Chapters covered; last search was on 1st June 2004. Searches of several commonly used literature databases have been performed, by industry and independent reviewers.References in Chemical Abstracts have been followed up in terms of citation, and relevant original references obtained from libraries. A report of the literature search methods and outcomes is available.
For full details of search strategy, refer to SIAR Section 7

04-AUG-2005

## 1.13 Reviews

**Remark:** Lington, A.W. and Bevan, C. 1994. Alcohols. In: Clayton, G.D. and Clayton, F.E. (eds.). Patty's Industrial Hygiene and Toxicology. vol. II, part D. New York: John Wiley & Sons, Inc. Pp. 2585-2760.

04-AUG-2005

## 2.1 Melting Point

**Value:** ca. 29 degree C

**Method:** other: (calculated) SRC MPBPVP v1.40
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Validation of melting point prediction using this method shows that the calculated values are close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.2 Boiling Point

**Value:** = 279 degree C

**Method:** other: (calculated) SRC MPBPVP v1.40
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Validation of boiling point prediction using this method shows that the calculated values are very close to the measurements for most carbon chain lengths. In the absence of reliable measured data, it is considered acceptable to use the value estimated by MPBPVP.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.3 Density

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** No measured data are available for this substance, and it is not possible to estimate with confidence what the relative density might be. However, it is notable that across the Category, measured density values at ambient temperatures range between approximately 0.80 - 0.85 g/cm3 (based on reliable values and those of non-assignable reliability).

The density for this substance would be expected to fall within this range.
**Reliability:** (4) not assignable
**Flag:** Critical study for SIDS endpoint
21-OCT-2005 (12)

## 2.3.1 Granulometry

-

## 2.4 Vapour Pressure

**Value:** = .00057 hPa at 25 degree C

**Method:** other (calculated): from composition
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** For all commercial alcohols, various chain lengths will be present, and the overall vapour pressure of the product has been calculated from the contribution (partial vapour pressure) of each component on a mole-% basis.
**Result:** Result = 5.7 X 10-4 hPa
**Reliability:** (2) valid with restrictions
The value was predicted using a partial vapour pressure contribution method, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.5 Partition Coefficient

**log Pow:** = 5.56 at 25 degree C

**Method:** other (calculated): amended SRC KOWWIN v1.66
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The SRC program KOWWIN and the number of carbon atoms have been used as inputs into a regression model, which fits the available data much better than KOWWIN alone.
**Remark:** The presence of branched components is not expected to significantly affect the predicted value.

Dissociation is not expected under normal conditions of pH (pKa expected to be >15).

A selection of accepted prediction methods were compared and the results were found to be in good agreement.
**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method supported by additional validation.
**Flag:** Critical study for SIDS endpoint
23-AUG-2005 (1)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .38 mg/l at 25 degree C

**Method:** other: (calculated) partition model
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the solubility reported represents the sum of the dissolved concentrations of all components. Therefore a standard method based on a partition model has been developed, validated and applied. A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4. Predictions of the individual concentrations are available in a confidential Annex to the SIAR.
**Remark:** Dissociation is not expected under normal conditions of pH (pKa expected to be >15).
**Result:** The water solubility is estimated to be 0.38 mg/l at a loading rate of 1000 mg/l.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
15-SEP-2005 (1)

## 2.6.2 Surface Tension

-

## 2.7 Flash Point

-

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

-

## 2.13 Viscosity

-

## 2.14 Additional Remarks

-

## 3.1.1 Photodegradation

**Method:** other (calculated): SRC AOPWIN v1.91
**Year:** 2004
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The rate constant of photodegradation in air has been estimated using the SRC AOPWIN program.
**Result:** Estimated rate constant: 19.8837E-12 cm3/molecule.sec
Half-life: 19.4 hours

The half-life is calculated from the rate constant, and assumes an OH radical concentration of 5E+05 OH molecules/cm3) (global average value, obtained from EU Technical Guidance for environmental risk assessment).

Linear components, present in the substance within the limits described in section 1.1-1.4, may be photodegraded slightly more slowly than branched components of equivalent carbon number, but the reported half-life represents a reasonable estimate for this substance.
**Reliability:** (2) valid with restrictions
This result was estimated using a standard calculation method, validated by limited measured data.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (3)

## 3.1.2 Stability in Water

**Remark:** This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal environmental conditions.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
15-SEP-2005

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Method:** other: Mackay Level I and Level III models
**Year:** 2005

**Result:** INPUT DATA USED:

Molecular weight 200.4
Data temperature 25 deg C
Log Kow 5.56
Water Solubility 0.38 mg/l
Vapour pressure 0.057 Pa
Melting point 29 deg C
half life in air 19.6 h
half life in water and soil 720 h
RESULTS:
The % environmental distribution calculated from the above parameters using the MacKay level 1 model is as follows:

| | |
|---|---|
| Air | 1.81% |
| Soil | 95.7% |
| Water | 0.30% |
| Fish | 5.39E-03% |
| Sediment | 2.13% |

The Level III program has also been used, with the default model, using the same input parameters. The distribution between compartments obtained is as follows:

| Release: | To air | To water | To soil |
|---|---|---|---|
| % in air | 67.4 | 0.016 | 0.00015 |
| % in water | 1.36 | 8.65 | 0.0117 |
| % in sediment | 14.3 | 91.3 | 0.123 |
| % in soil | 16.9 | 0.0040 | 99.9 |

The results reflect that the ultimate fate of tridecanol, branched and linear, is dependent on its route of release into the environment. Tridecanol, branched and linear released to air would partially precipitate to soil and water. There is relatively little
movement between soil and water, because transfer via the air compartment is very slow, for a substance of low volatility.

In water, the adsorption coefficient of tridecanol, branched and linear results in significant adsorption to sediment.

**Reliability:** (2) valid with restrictions
Assessment performed according to accepted models and principles.

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (4)

## 3.3.2 Distribution

**Media:** water - soil
**Method:** other (calculation): various methods
**Year:** 2004

**Method:** Various accepted methods were used to predict Koc. Neither of these approaches stands out in terms of reliability or performance. The value calculated by the TGD Non-hydrophobics equation is the most conservative across the category. The measured log Kow value of 5.51 was used in the TGD calculation methods.

**Result:**
TGD Hydrophobics method: Koc = 40100
TGD Non-hydrophobics method: Koc = 8150
TGD Alcohols method: Koc = 470

SRC PCKOCWIN method: Koc = 530

Note: the TGD Alcohols method is valid up to log Kow = 5. The result is presented for comparison only.

**Reliability:** (2) valid with restrictions
The value was predicted using accepted calculation methods.

29-DEC-2005 (3)

## 3.4 Mode of Degradation in Actual Use

-

## 3.5 Biodegradation

**Result:** other: Readily biodegradable meeting the 10 day window

**Method:** other: read-across based on grouping of substances (category approach)

**Year:** 2005

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** This substance is predicted to be readily biodegradable, meeting the ten-day window. This conclusion is drawn from analysis of trends in results measured in reliable studies for analogous substances (other Category members).

The presence of branched components in the substance, within the limits described in section 1.1-1.4, is not expected to affect the rate of biodegradability.

**Reliability:** (2) valid with restrictions
The value was predicted based on reliable data for similar substances. Refer to the category SIAR and IUCLID SIDS dossiers for relevant substances (listed in section 1.0.4 of this Dossier).

**Flag:** Critical study for SIDS endpoint

29-DEC-2005 (3)

## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

**BCF:** = 10600

**Method:** other: calculated (Veith et al, 1979)

**Year:** 2004

**GLP:** no

**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For substances with log Kow <6, the Veith et al linear equation was used to estimate BCF. For substances with log Kow >6, the parabolic recalculated Connell and Hawker equation was used. This approach is in accordance with standard EU recommendations.The measured log Kow value of 5.51 was used in the calculation.

**Remark:** Predicted values for branched alcohols suggest that

bioconcentration is expected to be slightly lower for branched structures than for linear alcohols of equivalent carbon number.The natural ability of biochemical systems in the body to metabolise alcohols may mean that predictions will tend to be overestimates.

**Reliability:** (2) valid with restrictions
The value was predicted using an accepted calculation method.

29-DEC-2005 (3)

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish

**Unit:** mg/l **Analytical monitoring:** no
**LC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

### 4.2 Acute Toxicity to Aquatic Invertebrates

**Unit:** mg/l **Analytical monitoring:** no
**EC50:** > 100

**Method:** other
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** For all commercial alcohols, various chain lengths will be present, and the loading rate reported represents the sum of the predicted effects of all components that have been modelled to dissolve in the medium. For complex liquid mixtures, a model of solubility and effects of the components was set up. The effects of the dissolved components are summed, and a 'loading rate' found which is predicted to give the LC50 (expressed as the lethal loading rate LL50). Based on this model, the properties of the mixture can be predicted.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using a multiple partitioning model, supported by additional validation.

**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (2)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Method:** other: read across/expert judgement
**Year:** 2005
**GLP:** no
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** The acute toxicity of essentially single carbon chain length alcohols has been estimated by expert judgement, with reference to measured and predicted results for other trophic levels.

Examination of the available measured data across the long chain alcohols Category suggests that algal EC50 values are of the same order of magnitude, or slightly lower, than the Daphnia EC50 values. However, there must always be uncertainty in such read across, so the estimated algal EC50 has been stated as a range. For this substance, the available Daphnia toxicity result is estimated by modelling.

A key input to this model is the compositional breakdown, which follows the description given in section 1.1-1.4.
**Result:** Predicted to be non-toxic at the limit of solubility.
**Reliability:** (2) valid with restrictions
The value was predicted using read across and expert judgement with validation based on measured data across the data set.
**Flag:** Critical study for SIDS endpoint
29-DEC-2005 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

-

## 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish

-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms

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### 4.6.2 Toxicity to Terrestrial Plants

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## 4.6.3 Toxicity to Soil Dwelling Organisms

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## 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species

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## 4.7 Biological Effects Monitoring

-

## 4.8 Biotransformation and Kinetics

**Remark:** Fatty alcohols can be metabolized by alcohol dehydrogenase and aldehyde dehydrogenase to fatty acids. Alcohol dehydrogenase is found in the soluble fraction of various tissues. The coenzyme is normally NAD, and although NADP may be utilized, the rate of the reaction is slower. The enzyme is relatively non-specific and so accepts a wide variety of substrates including exogenous primary and secondary alcohols, with primary alcohols being metabolized at a faster rate. The product of the oxidation is the corresponding aldehyde if the substrate is a primary alcohol or a ketone if a secondary alcohol is oxidized. The aldehyde produced by this oxidation may be further oxidized by aldehyde dehydrogenase to the corresponding acid. This enzyme also requires NAD and is found in the soluble fraction. Other enzymes may also be involved in the oxidation of aldehydes, particularly aldehyde oxidase and xanthine oxidase. These enzymes are primarily cytosolic, although microsomal aldehyde oxidase activity has been detected. They are flavoproteins, containing FAD and also molybdenum, and the oxygen incorporated is derived from water rather than oxygen. Aldehyde oxidase and xanthine oxidase both oxidize a wide variety of substrates. Occurence: The alcohol dehydrogenase enzyme system is ubiquitously present in the plant and animal kingdom. It has been specifically identified in man and in different species e.g. cod, fathead minnows, carp, eel, sardines, rainbow trout, rat, mice, and several plant sources. Aldehyde dehydrogenase is also ubiquitously present. First pass effect and main enzyme activity: In the caecum of freshwater gourami (Trichogaster cosby), metabolism of hexadecanol to hexadecanoic acid occurred during absorption. The first reaction in the sequence fatty alcohol-aldehyde-acid seems to occur under physiological conditions at a much slower rate than the second reaction so that free aldehyde is not detected. Also in rat, fatty alcohols are absorbed as fatty acids and fatty acid esters, particularly triglycerides. The highest alcohol dehydrogenase activity for rainbow trout and the carp is found in the liver, similar to organisms like man, rhesus monkey, horse, porpoise, rat, domestic fowl, frog and pike. In contrast, virtually all ADH in the goldfish is found in the red and white muscles. Rates and specificity: For a series of C4-C16 alcohols, the apparent Km values show a steady decrease with increasing hydrophobicity, whereas the maximum rates of oxidation remain similar. This suggests that

enzyme-substrate binding is governed largely by apolar interactions.

**Reliability:** (2) valid with restrictions
18-JAN-2006 (7)

## 4.9 Additional Remarks

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## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

**Remark:** Oral: Studies of DQ 1 or 2 all indicating acute oral LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-22). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, data for undecanol and C12-13 alcohols. This data supports the statement that Tridecanol is expected to be of low acute oral toxicity LD50 >2000 mg/kg.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (14)

### 5.1.2 Acute Inhalation Toxicity

**Remark:** Studies of DQ 2 supported by secondary and/or literature references (DQ4) over the carbon range of this category C6-20 suggest that these alcohols are of a low order of acute inhalation toxicity with the LC50 in excess of the saturated vapour concentration. This includes data for C11 (undecanol), C12-16 and tridecanol (Cas 112-70-9) alcohols in support of the statement that Tridecanol branched and linear Cas 90583-91-8 alcohols are expected to be of a low order of acute inhalational toxicity with the LC50 in excess of the saturated vapour concentration.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** The LC50 is expected to be greater than the substantially saturated vapour concentration.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (14)

### 5.1.3 Acute Dermal Toxicity

**Remark:** Studies of DQ 1 or 2 all indicating acute dermal LD50 values in excess of 2000 mg/kg are available over the carbon range of the category (C6-20). This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, data for undecanol and C12-13 alcohols. This data supports the statement that Tridecanol is expected to be of

low acute dermal toxicity LD50 >2000 mg/kg.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Expected to be of low toxicity LD50 >2000 mg/kg.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (14)

### 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

### 5.2.1 Skin Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. For the subcategory of essentially linear alcohols, of which Tridecanol (branched and linear Cas 90583-91-8) is a member, the skin irritation potential for the higher members in the range C12 - C16 is mild - essentially non-irritant. This includes data reported for 1-tridecanol (Cas 112-70-9) on a sample described as mixed isomers, together with data on C12-13 and C12-16 alcohols. This supports the conclusion that Tridecanol (branched and linear, Cas 90583-91-8) is expected to be mildly irritating to the skin.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Tridecanol (branched and linear) is expected to be mildly irritating to the skin.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
11-MAY-2006 (14)

### 5.2.2 Eye Irritation

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category C6-22. The evidence indicates that lower chain members (C6-11) of the category (linear and essentially linear) are eye irritants while alcohols of chain length >C12 are essentially non-irritating to the eye. Data available for C12-13 and C12-15 alcohols support the conclusion that tridecanol (branched and linear) alcohol is expected to be essentially non-irritating to the eye.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Tridecanol (branched and linear) is expected to be essentially non-irritating to the eye.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (14)

## 5.3 Sensitization

**Remark:** Test data DQ 1 or 2 are available over the carbon range of this category from C6-C18. Included are negative data from guinea pig maximisation tests for C10-16 (Types B&C), C12 (dodecanol), C12-16 (Type A), C14-16 (type A) and C16 (hexadecanol) alcohols which support the conclusion that Tridecanol (branched and linear) alcohols are not expected to be skin sensitisers.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** Not expected to be a skin sensitiser.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.
05-DEC-2005 (14)

## 5.4 Repeated Dose Toxicity

**Remark:** There are no significant toxicological effects, following repeated exposure, for the category as a whole. Data in support of this statement for tridecanol (linear and branched) alcohols, from studies in experimental animals of at least 28 days duration and of reliability 1 or 2, are available for 1-dodecanol (supporting), C10-16 alcohols (Type B), C14-16 alcohols (type B) and 1-hexadecanol . The oral NOAELs for these studies are all in excess of 100 mg/kg for a 90 day study (or 300 mg/kg/day for a 28 day study).

This data together with information from studies involving shorter exposure periods and/or investigating specific systemic endpoints supports the conclusion presented in the Human Health Effects chapter of the Aliphatic Alcohols Category SIAR that members of the category of aliphatic alcohols are of a low order of toxicity upon repeated exposure.
**Test substance:** as prescribed by 1.1 - 1.4
**Conclusion:** ected to be of low systemic toxicity on repeated exposure.
**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment
15-SEP-2005 (10) (14)

## 5.5 Genetic Toxicity 'in Vitro'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro testing over the carbon range (C6-22) of category members (linear and essentially linear) and supporting substances (C5-C24-34) provides evidence for the lack of mutagenic activity. Negative data in support of this conclusion for tridecanol (branched and linear) are available from studies of

reliability 1 or 2 for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vitro.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (10) (14)

## 5.6 Genetic Toxicity 'in Vivo'

**Remark:** The category members contain no structural elements which may be of concern for potential mutagenic activity. In vitro tests over the carbon range (C6-22) of the category members (linear and essentially linear) and supporting substances (C5 to 24-34) including data for 1-decanol [Ames], C10-16 alcohols (types B&C) [Ames, chromosome aberration, gene conversion], C12-16 (types A&B), 1-dodecanol and tetradecanol [Ames] are negative.

Evidence from in vivo studies on other category members supports the conclusion that these alcohols are not genotoxic in vivo. Negative data of reliability 1 or 2 in support of this conclusion are available for 2-ethyl hexanol (supporting) [negative dominant lethal, micronucleus and chromosome aberration studies], 1-dodecanol and 1-octadecanol (supporting) [negative micronucleus assays], docosanol [negative micronucleus assay], C24-32 alcohols (supporting) [negative micronucleus and dominant lethal assays].

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be genotoxic in vivo.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are guideline or comparable studies or publications with sufficient detail for assessment.

15-SEP-2005 (8) (10) (11) (14)

## 5.7 Carcinogenicity

-

## 5.8.1 Toxicity to Fertility

**Remark:** The conclusion that the members of the aliphatic alcohol category (C6-22) are not expected to impair fertility is based on a weight of evidence approach using negative data from reproductive screening studies [C12 (dodecanol), C18 (octadecanol)] and a fertility study [C22 (docosanol)] together with a lack of effect on the reproductive organs in repeat dose studies over the range of linear and essentially linear alcohols.

Data in support of the conclusion that tridecanol (branched

and linear) is not expected to impair fertility are provided, in addition to the reproduction/fertility studies mentioned above, by lack of effects on the reproductive organs of rats receiving 1-hexanol, C6-12 alcohols (type C), C10-16 alcohols (types B&D), C14 -16 (type A) and data from supporting substances 1-hexanol-2-ethyl and isoamyl alcohol.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to impair fertility.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (8) (14)

## 5.8.2 Developmental Toxicity/Teratogenicity

**Remark:** Representative data are available for the subcategory of linear alcohols, covering the low (C6, C8, C9), intermediate (C10, C12) and high (C18, C22 and higher) carbon chain lengths of this class. For the essentially linear alcohols, the key data are derived from the supporting substances isoamyl alcohol and C7-11 alcohol [CAS 85566-14-9], consisting of C7, C9 and C11 alcohol (65% linear). The available test data indicate that for both linear and essentially linear alcohols there is no evidence of foetotoxicity in the absence of maternal toxicity and supports the conclusion that tridecanol (branched and linear) is not expected to be a developmental toxicant in the absence of maternal toxicity.

**Test substance:** as prescribed by 1.1 - 1.4

**Conclusion:** Not expected to be a developmental toxicant in the absence of maternal toxicity.

**Reliability:** (2) valid with restrictions
The studies on which the conclusion is based are comparable to guideline studies or publications with sufficient detail for assessment

15-SEP-2005 (10) (11) (14)

## 5.8.3 Toxicity to Reproduction, Other Studies

-

## 5.9 Specific Investigations

-

## 5.10 Exposure Experience

-

## 5.11 Additional Remarks

-

(1) Annex I (2005). Physico-chemical properties: Measured values and QSAR predictions; Annex I to the Long Chain Aliphatic Alcohols SIAR.

(2) Annex IX (2005). Ecotoxicology: Interpretation of data for multi-component substances; Annex IX to the Long Chain Aliphatic Alcohols SIAR.

(3) Annex V (2005). Environmental Fate Data: QSAR predictions and comparison with measured values; Annex V to the Long Chain Aliphatic Alcohols Category SIAR.

(4) Annex VI (2005). Environmental Distribution Modelling; Annex VI to the Long Chain Aliphatic Alcohols Category SIAR.

(5) Annex VIII (2005). Ecotoxicology: QSAR predictions and comparison with measured values; Annex VIII to the Long Chain Aliphatic Alcohols SIAR.

(6) APAG/CEFIC annual statistical data; APAG Alcohols Group; Total consumption, year 2004, CEFIC statistics service.

(7) de Wolf, W. and Parkerton, T. 1999. Higher alcohols bioconcentration: Influence of biotransformation. Preprints of Extended Abstracts 39:101-103. Presented in the session Persistent, Bioaccumulative, Toxic Chemicals: Food Chain Transfer and exposure, part 1 at the American Chemical Society Symposium, Anaheim, CA March 21-25, 1999.

(8) IPCS/WHO 1993 Toxicological evaluation of certain food additives and contaminants. 2-ethyl hexanol WHO Food Additives Series 32 pp 35-55.

(9) Modler RF, Gubler R, and Inoguchi Y.; Detergent Alcohols. In: Chemical Economics Handbook Marketing Research Report. SRI International, Menlo Park, CA USA, 2004.

(10) SIDS Dossier - Dodecanol, 1998 with additional robust summaries for studies for key endpoints provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005

(11) SIDS Dossier - Octadecanol, 1995 with additional robust summaries for studies for key end points provided by consortium members, prepared in support of the Aliphatic Alcohols category on behalf of the Global ICCA Aliphatic alcohols Consortium, 2005.

(12) SIDS Initial Assessment Report for Long Chain Alcohols (C6-22 primary aliphatic alcohols) Category, 2005

(13) US IUR ('Inventory Update Rule') volumes; Toxic Substances Control Act (TSCA) Chemical Inventory data base; sourced via the US EPA website.

(14) Veenstra, G.; Webb, C 2005 Health effects SIAR for Long Chain Alcohols (C6-22) including Iuclid dossiers chapter 5 prepared for the Aliphatic Alcohols category

# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 123-51-3 |
| **CAS No.** | **:** | 123-51-3 |
| **EINECS Name** | **:** | 3-methylbutan-1-ol |
| **EC No.** | **:** | 204-633-5 |
| **Molecular Formula** | **:** | C5H12O |

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**Remark** : The authors summarise literature data available for isoamyl alcohol. This data suggests that primary amyl alcohols are mainly oxidised to the corresponding valeric acids via the aldehyde. Following a dose of 1g/kg of isoamyl alcohol only 0.97% was excreted unchanged in the expired air and 0.27% in the urine of rats. Valeraldehyde was detected in the blood of rats after intraperitoneal doses of n-amyl alcohol. Evidence suggested that oxidation occurred in the liver. As clinical effects persisted after both alcohol and aldehyde were no longer detectable in the blood the presence of some other metabolite was postulated.

In rabbits 9% of an oral dose of isoamyl alcohol was excreted as a glucuronide in the urine within 24 hours.

**Reliability** : (2) valid with restrictions

**Source** : Carpanini et al, 1973
Hayes Consultancy Service Bromley, Kent

20.07.2005 (2)

## 5.1.1 ACUTE ORAL TOXICITY

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

## 5.2.2 EYE IRRITATION

## 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | male/female |
| **Strain** | : | other: Ash/CSE |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 3, 6 or 17 weeks |
| **Frequency of treatment** | : | daily |
| **Post obs. period** | : | none |

| | | |
|---|---|---|
| **Doses** | : | 0, 150, 500 and 1000 mg/kg bw |
| **Control group** | : | yes, concurrent vehicle |
| **NOAEL** | : | = 500 mg/kg bw |
| **LOAEL** | : | = 1000 mg/kg bw |
| **Method** | : | other: see text |
| **Year** | : | 1972 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : C5 alcohol Cas no. 123-51-3 >=98% pure source N.V. Chemische Fabriek Naarden, Netherlands

**Test condition** :

TEST ORGANISMS
- Age: not reported
- Weight at study initiation: M 80-115g; F 80-105g
- Number of animals: 15M+15F for 17 weeks plus groups of 5M+5F for 3 and 6 weeks.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 3, 6 and 17 weeks
- Type of exposure: gavage
- Post exposure period: none
- Vehicle: corn oil
- Concentration in vehicle: Adjusted to give constant dosing volume
- Total volume applied: 5 ml/kg
- Doses: 0, 150, 500 and 1000 mg/kg bw

SATELLITE GROUPS AND REASONS THEY WERE ADDED: 5M+5F at each dose level received the test compound at doses of 0, 500 and 1000 mg/kg for 3 or 6 weeks. These groups were used to provide interim blood samples and organ weights .

An additional study was carried out to investigate the organ weights changes observed in males rats after 3 weeks dosing. 3 groups of 8 litter mate trios each were given: A- 5 ml/kg corn oil for 3 weeks with ad lib feeding. B-1000 mg/kg isoamyl alcohol in 5 ml/kg corn oil and fed ad-lib C- 5 ml/kg corn oil alone but pair-fed with its isoamyl alcohol treated litter mate so that the food consumed by these two groups was equal.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Not reported
- Mortality: Not reported
- Body weight: Main study weekly
- Food consumption: Main study days weekly
- Water consumption: Main study weekly
- Ophthalmoscopic examination: Not reported
- Haematology: Week 3, 6 and 17 (Hb, PCV, RBC, Retics % RBC, Leucocytes (total & differential)
- Biochemistry: Week 3, 6 and 17 (serum urea, total protein & albumin, ALAT, ASAT, GPT, LDH) Fasting blood taken from the aorta.
- Urinalysis: Week 3, 6 and 17 (appearance, specific gravity, cells, glucose, ketones, bile salts, blood) Also a dilution & concentration test carried out.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: Brain, heart, liver, spleen, kidneys, stomach, small intestine, caecum, adrenals, gonads, pituitary, thyroid
- Macroscopic: As above plus lung, lymph nodes, salivary gland, trachea, oesophagus, aortic arch, thymus, urinary bladder, colon, rectum, pancreas, uterus, skeletal muscle.

- Microscopic: Microscopic examination was carried out on all the above listed organs for half of the controls and all top dose level animals. Additionally tissues exhibiting macroscopic anomalies were examined.

STATISTICAL METHODS: Student's T test

**Result** **:** NOAEL (NOEL): 500 mg/kg/day; LOAEL (LOEL): 1000 mg/kg/day based on a significant decrease in body weight in top dose males.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
M&F 150, 500 & 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: 1000 mg/kg One male died at week 8 and one female at week 10. Histopathological examination confirmed that these deaths were consistent with misdosing by the intratracheal route.

- Clinical signs: Behaviour was reported as normal throughout the study for all survivors.

- Body weight gain: At 17 weeks male rats receiving 1000 mg/kg showed a significant decrease (9%) in body weight gain compared to controls. The reduction was significant from week 9 onwards. There were no other significant changes in body weight gain.

- Food/water consumption: There were no significant differences in mean food intake over the period of the study despite some reduction in top dose rats in the early part of the study. Water consumption was unaffected by treatment.

- Ophthalmoscopic examination: Not carried out.

- Clinical chemistry: There were no significant differences in any of the parameters monitored.

- Haematology: The were no significant differences between treated and control animals. Isolated increases in PCV, Hb and RBC at weeks 3 & 6 were neither sex nor dose related.

- Urinalysis: The were no significant differences between treated and control animals.

- Organs weights: At 17 weeks there were no significant effects on absolute or relative organ weights in male and female rats at any dose level. The only effect at 6 weeks was decreased absolute pituitary weight in top dose male rats. At 3 weeks there were no significant effects on female organ weights at any dose level while in top dose males at 3 weeks most absolute organ weights were significantly reduced. At 500 mg/kg significant reduction in absolute brain, kidney, stomach, small intestine and testes weights were seen in males only. When these organ weights were expressed relative to body weight the only significant effect was found in the testes at both 500 and 1000 mg/kg.

- Gross and histopathology: There were no treatment related changes in gross or microscopic pathology. Small testes observed in 3 males after 3 weeks were not accompanied by histopathological change. One female receiving 500 mg/kg for 17 weeks developed a lipoma of the salivary gland but this was not considered treatment related as this was an isolated incidence and such lesions are reported to occur spontaneously with an

incidence of 2-3%.

- Other: Further investigation of the organ weight changes in males after 3 weeks dosing showed a slight reduction in weight gain compared to ad-lib fed controls but the rate of body weight gain was similarly reduced in pair fed control animals. The organ weights of all 3 groups was similar. This indicates that the effects on organ weights (testes) seen in the main study at 3 weeks only was probably a reflection of the difference in body weight.

STATISTICAL RESULTS: Students T test.

**Conclusion** : The NOAEL for this 17 week rat gavage study was 500 mg/kg/day based on a 9% reduction in body weight in top dose males. This reduced body weight gain at the 1000 mg/kg level was due to reduced food intake in the early weeks of the study.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

20.07.2005 (1) (2)

## 5.5 GENETIC TOXICITY 'IN VITRO'

## 5.6 GENETIC TOXICITY 'IN VIVO'

## 5.7 CARCINOGENITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | other: SPF-Wistar |
| **Route of admin.** | : | inhalation |
| **Exposure period** | : | day 6-15 postcoitum |
| **Frequency of treatment** | : | 6 hr/day |
| **Duration of test** | : | 20 days |
| **Doses** | : | 0.5, 2.5 and 10 mg/L |
| **Control group** | : | yes |
| **NOAEL Maternalt.** | : | = 2.5 mg/l |
| **NOAEL Teratogen** | : | = 10 mg/l |
| **Method** | : | other: see text |
| **Year** | : | 1992 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** : TEST ORGANISMS:
Female rats (Wistar) weighing approx 216 g at the starat of the experiment aged 10-11 weeks. Groups of 25 rats were mated at each dose level.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored hourly.

- Duration of test/exposure: Days 6-15 post coitum
- Doses: 0. 0.5, 2.5 or 10 mg/l 6 hours/day

MATING PROCEDURES: 4 females mated with one male.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: recorded day 0, 3, and 6 then every 3 days until day 20 post coitum.
- Food consumption: Not reported
- Clinical observations: Daily
- Examination of uterine content: Day 20 post coitum uterine weight, number of implants, live and dead implants, % pre and post implantation loss.
- Ovaries: Number of corpora lutea
- Examination of fetuses: Mean foetal weight, sex ratio, mean palcental weight. external, soft tissue and skeletal malformations and variations/retardations were recorded

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Macroscopic examination of dams. no histopathological examinations carried out.

STATISTICAL METHODS: Dunnett test and Fischers exact test.

**Result** **:** NOAEL: Maternal toxicity 2.5 mg/l; foetal toxicity 10 mg/l.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0.51, 2.5 and 9.8 mg/l

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: One non-pregnant low dose rat died on day 12 post coitum.
- Number pregnant per dose level: Controls 22/25; 0.5 mg/l 20/25; 2.5 mg/l 25/25; 10 mg/l 23/25. No significant differences between treated and control groups.
- Number aborting: None
- Number of implantations: No significant differences between treated and control groups. Implants/dam 13.6, 13.9, 14.5 and 15.6 for controls, low, mid and high dose respectively.

- Pre and post implantation loss: No significant differences between treated and control groups. Preimplantation loss 8.7, 12.5, 7.2 and 3.3% Postimplantation loss 10.3, 10.0, 6.8 and 9.3% for controls, low, mid and high dose respectively.
- Number of corpora lutea: No significant differences between treated and control groups. Corpora lutea/dam 15.5, 15.9, 15.6 and 16.3 for controls, low, mid and high dose respectively.- Body weight: No significant effect on body weight or body weight gain in the lower treatment groups. Top dose rats (10 mg/l) showed a statistically significant decrease in body weight gain ($p<0.05$) over days 6-9 [Control bodyweight change 13.4; Top dose body weight change 9.9g*] and an increased bodyweight gain ($p<0.01$) between days 12-15. There was no clear dose relationship for these changes.
- Description, severity, time of onset and duration of clinical signs: None.
- Hematological findings incidence and severity: Not recorded
- Clinical biochemistry findings incidence and severity: Not recorded
- Gross pathology incidence and severity: Comparable between treated and control groups.
- Organ weight changes: No difference between treated and control groups

in uterine or placental weight. No other organs weighed.
- Histopathology incidence and severity: Not carried out.

FETAL DATA: No significant differences between treated and controls.
- Litter size and weights; number viable; sex ratio: No significant differences between treated and control groups. Litter size 13.4, 12.6, 13.5 and 14.2 live foetuses/dam; mean foetal weights 3.9, 3.9, 4.0 and 3.8 gm; sex ratio (male:female)50:50, 49:51, 51:49 and 51:49 for controls, low, mid and high dose respectively.
- External abnormalities: Polydactyly was observed in 1/326 foetuses examined at the top dose level (10 mg/kg/day). No external variations were observed.
- Soft tissue abnormalities: Dilatation of the ventricles and dextrocardia were each observed in 1/160 foetuses examined at the mid dose (2.5 mg/kg/day). Soft tissue variations occurred in all groups including controls in particular dilated renal pelvis and hydro-ureter. These findings were independent of exposure or dose level.
- Skeletal abnormalities: There were various malformations of the sternebrae and/or vertebral column none of which were of statistical significance. Variations and retardations were seen in all groups but there were no significant differences.

**Conclusion** : The NOAEL for foetotoxicity and teratogenicity in rats, following inhalation exposure to isoamyl alcohol on gestation days 6-15, is 10 mg/l (highest dose level). There were no statistically significant differences in maternal reproductive or foetal parameters investigated between controls and treated groups at any dose level. The NOAEL for maternal toxicity is considered to be 2.5 mg/l based on retardation of maternal weight gain during gestation (days 6-9).

**Reliability** : (2) valid with restrictions
**Source** : Klimisch, 1995
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
09.01.2006 (3)

**Species** : rabbit
**Sex** : female
**Strain** : Himalayan
**Route of admin.** : inhalation
**Exposure period** : days 7-19 postinsemination
**Frequency of treatment** : 6 hours/day
**Duration of test** : 29 days
**Doses** : 0.5, 2.5 and 10 mg/l
**Control group** : yes
**NOAEL Maternalt.** : = 2.5 mg/l
**NOAEL Teratogen** : = 10 mg/l
**Method** : other: see text
**Year** : 1992
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS:
Female rabbits (Himalayan) weighing approx 2.5 - 2.7 kg at the start of the experiment aged 24-29 weeks. Groups of 15 rabbits were mated at each dose level.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored hourly.
- Duration of test/exposure: Days 6-15 post coitum
- Doses: 0. 0.5, 2.5 or 10 mg/l 6 hours/day

MATING PROCEDURES: artificial insemination.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: recorded day 0, 3, and 7 then every 3 days until day 29 postinsemination.
- Food consumption: Not reported
- Clinical observations: Daily
- Examination of uterine content: Day 29 post coitum uterine weight, number of implants, live and dead implants, % pre and post implantation loss.
- Ovaries: Number of corpora lutea
- Examination of fetuses: Mean foetal weight, sex ratio, mean palcental weight. external, soft tissue and skeletal malformations and variations/retardations were recorded

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Macroscopic examination of dams. no histopathological examinations carried out.

STATISTICAL METHODS: Dunnett test and Fischers exact test.

**Result** **:** NOAEL: Maternal toxicity 2.5 mg/l based on growth retardation of the dams; foetal toxicity 10 mg/l (highest dose level tested).

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0.51, 2.51 and 9.8 mg/l

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Controls 14/15, all treated groups 15/15.
- Number aborting: 1 at the 0.5 mg/l group and 1 at the top dose level (10 mg/l).
- Number of implantations: No significant differences between treated and control groups. Implants/dam 6.8, 6.9, 7.5 and 7.8 for control, low, mid and high dose groups respectively.
- Pre and post implantation loss: No significant differences between treated and control groups. Preimplantation loss 20.3, 17.1, 17.7 and 3.3%; postimplantation loss 18.4, 8.5,
10.0 and 10.7% for control, low, mid and high dose groups respectively.
- Number of corpora lutea: No significant differences between treated and control groups. Corpora lutea/dam 8.4, 8.3, 9.0 and 8.1 for control, low, mid and high dose groups respectively.
- Body weight: No significant effect on body weight or body weight gain at 0.5 and 2.5 mg/l. At the top dose level (10 mg/l) there was a slight retardation in body weight gain throughout the exposure period which reached statistical significance ($p<0.05$) between days 7-10. [control body weight change days 7-10 15g; top dose bodyweight change -17.5g*]
- Description, severity, time of onset and duration of clinical signs: Eye irritation in top dose animals only occuring during exposure. No other clinical signs.
- Hematological findings incidence and severity: Not recorded
- Clinical biochemistry findings incidence and severity: Not recorded
- Gross pathology incidence and severity: Comparable between treated and control groups.
- Organ weight changes: No difference between treated and control groups in uterine or placental weight. No other organs weighed.
- Histopathology incidence and severity: Not carried out.

FETAL DATA: No significant differences between treated and controls. Slight reductions (non-significant) in foetal weights were due to the incidental increase in live foetuses/dam in treated compared to control groups.
- Litter size and weights; number viable; sex ratio: No significant differences between treated and control groups. Live foetuses/dam 5.6, 6.3, 6.7 and 6.9; mean foetal weight 41.3, 40.6, 40.0 and 39.3; sex ratio (male:female) 42:58, 46:54, 52:48 and 41:59 for control, low, mid and high dose groups respectively.
- External abnormalities: No external malformations, one type of variation (pseudoankylosis) was observed in 0/79 controls, 1/96 foetuses at 0.5 and 1/100 at 2.5 mg/l and in 2/103 foetuses at 10 mg/kg/day. This was a similar incidence to that seen in historical controls 14/1348.
- Soft tissue abnormalities: No malformations. There was an increased incidence of a commonly occurring variation 'separated origin of carotid' which attained statistical significance ($p<0.05$) at the top dose level on both a litter and foetus basis (29/103 foetuses 28.2%; 13/15 litters 86.7%). However this was within historical control limits (% foetuses with malformation 10.3-75%, litter incidence 47.4-100%) and additionally the study control incidence values of 13.9% of foetuses and 21.45 litters was low so htat the finding was considered incidental.
- Skeletal abnormalities: There were various malformations of sternebrae and/or vertebral column, variations of the vertebral column, sternum & ribs and retardations observed in all treatment and control groups, none reaching statistical significance.

**Conclusion** : NOAEL for maternal toxicity in rabbits, following inhalation exposure to isoamyl alcohol on gestation days 7-19, is 2.5 mg/l based on body weight retardation during pregnancy (days 7-10). The NOAEL for foetotoxicity and teratogenicity is considered to be 10 mg/l (top dose level). The increased incidence in some foetal malformations and/or variations and retardations were within historical control ranges. All other reproductive and developmental indices were comparable between treated and control groups.

**Reliability** : (2) valid with restrictions

**Source** : Klimisch, 1995
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

09.01.2006 (3)

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

(1) Carpanini, F, I Gaunt, I Kiss, P Grasso and S Gangolli. 1972. Short-term toxicity of isoamyl alcohol in rats. BIBRA Research Report No. 6/1972.

(2) Carpanini, F, I Gaunt, I Kiss, P Grasso and S Gangolli. 1973. Short-term toxicity of isoamyl alcohol in rats. Fd. Cosmet. Toxicol. 11:713-724.

(3) Klimisch, HJ and J Hellwig. 1995. Studies on the prenatal toxicity of 3-methyl-1-butanol and 2-methyl-1-propanol in rats and rabbits following inhalation exposure. Fundamental and Applied Toxicology. 27, 77-89.

# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

Note: References in this file are given separately for physicochemical properties, environmental fate, ecotoxicology (i.e. chapters 2-4) and human health endpoints (chapter 5).

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 111-70-6 |
| **CAS No.** | **:** | 111-70-6 |
| **EINECS Name** | **:** | heptan-1-ol |
| **EC No.** | **:** | 203-897-9 |
| **Molecular Formula** | **:** | C7H16O |

## 2.1 MELTING POINT

**Value** : = -34 °C
**Sublimation** :
**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Verschueren 1996.
**Reliability** : (4) not assignable
24.09.2003 (12)

## 2.2 BOILING POINT

**Value** : = 176 °C at
**Decomposition** :
**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Budavari 1996.
**Reliability** : (4) not assignable
24.09.2003 (6)

## 2.3 DENSITY

**Type** :
**Value** : = .82 at °C
**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Verschueren 1996.
**Reliability** : (4) not assignable
24.09.2003 (12)

## 2.4 VAPOUR PRESSURE

**Value** : = .28 hPa at 25 °C
**Decomposition** :
**Method** : other (measured)
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Daubert and Danner 1989.
**Reliability** : (2) valid with restrictions
30.09.2003 (7)

**Value** : = .29 hPa at 25 °C
**Decomposition** :
**Method** : other (measured)
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : SRC.
**Reliability** : (4) not assignable
24.09.2003 (9)

**Value** : = 1.33 hPa at 42 °C
**Decomposition** :
**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Verschueren 1996.
**Reliability** : (4) not assignable
24.09.2003 (12)

## 2.5 PARTITION COEFFICIENT

**Partition coefficient** : octanol-water
**Log pow** : = 2.57 at °C
**pH value** :
**Method** : other (measured)
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Method** : The generator column was coated with liquid solute and 1-octanol. Water was then pumped into the column. Analysis of the aqueous phase from the 1% octanol coated column was used to determine the Kow.
**Source** : Tewari et al. 1982.
**Reliability** : (2) valid with restrictions
19.08.2003 (10)

**Partition coefficient** : octanol-water
**Log pow** : = 2.62 at °C
**pH value** :
**Method** : Other (measured)
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : SRC.
**Reliability** : (4) not assignable
24.09.2003 (9)

## 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water
**Value** : = 900 mg/l at 18 °C
**pH value** :

| | | |
|---|---|---|
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Source** | : | Verschueren 1996. |
| **Reliability** | : | (4) not assignable |

29.10.2003 (12)

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 1313 mg/l at 20 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Method** | : | A generator column was coated with liquid solute. Water was pumped into the column. Analysis of the aqueous phase from the pure solute coated column yielded the aqueous solubility. |
| **Source** | : | Tewari et al. 1982. |
| **Reliability** | : | (2) valid with restrictions |

29.10.2003 (10)

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 1670 mg/l at 25 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other: (measured) |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Source** | : | SRC. |
| **Reliability** | : | (4) not assignable |

24.09.2003 (9)

## 3.5 BIODEGRADATION

| | | |
|---|---|---|
| **Type** | : | aerobic |
| **Inoculum** | : | activated sludge |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Method** | : | Incubation was carried out in 200 ml Erlenmeyer flasks containing 5 ul of a alcohol and 100 ml of medium. Biodegradation rate constant was calculated from the time-course of the alcohol concentration in the supernatant of the culture. The concentration was analysed by gas chromatography. |
| **Result** | : | The biodegradation rate constant for Heptanol was 0.124 hr-1. This equates to a half-life of 5.6 hours. |
| **Source** | : | Yonezawa and Urushigawa 1979. |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

18.09.2003 (13)

## 3.6 BOD5, COD OR BOD5/COD RATIO

| | | |
|---|---|---|
| **BOD5** | | |
| **Method** | : | other: APHA 1980 |
| **Year** | : | |
| **Concentration** | : | related to |
| **BOD5** | : | mg/l |
| **GLP** | : | no data |
| **Method** | : | Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical. |
| **Remark** | : | The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols. |
| **Result** | : | 56.3% degradation after 5 days (% ThOD) |
| **Source** | : | Vaishnav et al. 1987. |
| **Test substance** | : | Heptanol (111-70-6) |
| **Reliability** | : | (2) valid with restrictions |

13.08.2003 (11)

## AQUATIC ORGANISMS

### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | flow through |
| **Species** | : | Pimephales promelas (Fish, fresh water) |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **LC50** | : | = 37.9 |
| **Limit test** | : | no |
| **Analytical monitoring** | : | yes |
| **Method** | : | other: ASTM 1980 |
| **Year** | : | 1985 |
| **GLP** | : | no data |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Remark** | : | Flow-through toxicity tests were conducted with a geometric series (0.8 dilution factor) of toxicant concentrations for all tests. Test water was maintained at 25 C and pH 7.6. Five fry or juveniles were added to each treatment and control chamber, providing a total of 20 test organisms per treatment level.<br>The test was performed in 1985. |
| **Result** | : | RESULTS: EXPOSED<br>LC50 = 37.9 mg/l for fry<br>Based on measured concentrations<br>RESULTS: CONTROL<br>Number/% showing adverse effects: No control mortality in tests with juveniles and less than 10% in tests with fry (refers to all 27 chemicals tested in study) |
| **Source** | : | Broderius et al. 1985. |
| **Test condition** | : | TEST ORGANISMS<br>Strain: Fathead minnow<br>Supplier: Not reported<br>Age: Newly hatched fry were < 24 hours old<br>Weight: not reported<br>Feeding: Spawning stock and juveniles were cultured on recently hatched brine shrimp nauplii (Artemia sp.) and frozen adult brine shrimp<br>Pretreatment: Acclimated to test chambers for 2-3 hours prior to introduction of toxicants<br>Feeding during test: none<br>Control group: 5 replicates<br>STOCK AND TEST SOLUTION AND THEIR PREPARATION<br>Vehicle: not reported<br>Concentration of vehicle/solvent: not reported<br>STABILITY OF TEST CHEMICAL SOLUTIONS<br>not reported<br>DILUTION WATER<br>Source: Lake Superior<br>Aeration: Aeration in head water reservoirs<br>Alkalinity: 44.0 mg/L as CaCO3<br>Hardness: 44.6 mg/l<br>Conductance: not reported<br>TEST SYSTEM<br>Concentrations: not reported but publication indicates daily analytical monitoring was conducted<br>Renewal of test solution: water replacement 2-4 h (25mL/min)<br>Exposure vessel type: Glass with silicone sealant |

Number of replicates: 1
Fish per replicate: 5
Test temperature: mean 25C
Dissolved oxygen: above 80% saturation
pH mean: 7.6
Adjustment of pH: not reported
Intensity of irradiation: 22 to 38 lumens/sq ft
Photoperiod: Illuminated with wide spectrum fluorescent bulbs for 16 h daily
TEST PARAMETER: lethality
SAMPLING: moralities recorded daily
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.08.2003 (5)

**Type** : static
**Species** : Alburnus alburnus (Fish, estuary)
**Exposure period** : 96 hour(s)
**Unit** : mg/l
**LC50** : = 45
**Limit test** : no
**Analytical monitoring** : no data
**Method** : other
**Year** : 1984
**GLP** : no data
**Test substance** : other TS: Heptanol (111-70-6)

**Remark** : This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
The earlier study reports the LC50 = 42-49 mg/l

**Result** : RESULTS: EXPOSED
LC50 = 45 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported

**Source** : Bengtsson, 1984
**Reliability** : (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available
18.08.2003 (1) (8)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Type** : static
**Species** : Daphnia magna (Crustacea)
**Exposure period** : 24 hour(s)
**Unit** : mg/l
**EC0** : = 62
**EC50** : = 82
**EC100** : = 100
**Limit Test** : no
**Analytical monitoring** : no
**Method** : other
**Year** : 1982
**GLP** : no

**Test substance** : other TS: Heptanol (111-70-6)
**Remark** : Bringmann and Kuhn 1977 reported a single value of 94 mg/l which appears to have been reworked in this 1982 paper.
**Result** : RESULTS: EXPOSED
EC0: 62 mg/l
EC50: 82 (79-85 mg/l)
E100: 100 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source** : Bringmann and Kuhn 1982.
**Test condition** : TEST ORGANISMS
Strain: Daphnia magna
Supplier: Laboratory culture
Age: <24hrs old
Feeding: Dry algae
Pretreatment: None
Feeding during test: Not reported
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF THE TEST CHEMICAL SOLUTIONS: no analysis
DILUTION WATER
Source: Standardised synthetic fresh water
Aeration: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Range of test concentrations to achieve three or more responses between 0 and 100%
Renewal of test solution: none
Exposure vessel type: 50 ml flask
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 20 C
Dissolved oxygen: oxygen saturated
pH mean: 7.6 - 7.7
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: 9 hours artificial lighting
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:
None
**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
14.08.2003 (4)

**Type** : static
**Species** : Nitocra spinipes (Crustacea)
**Exposure period** : 96 hour(s)
**Unit** : mg/l
**LC50** : = 169 - 210
**Limit Test** : no
**Analytical monitoring** : no data
**Method** : other:
**Year** : 1979
**GLP** : no data
**Test substance** : other TS: Heptanol (111-70-6)

| | | |
|---|---|---|
| **Method** | : | The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C. |
| **Remark** | : | This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail. |
| **Result** | : | Initial test, Heptanol was dissolved in water only. The LC50 = 210 mg/l. Due to low water solubility of alcohols they were also dissolved in redistilled acetone. By this method the LC50 = 169 mg/l. |
| **Source** | : | Bengtsson, 1984 |
| **Reliability** | : | (2) valid with restrictions<br>Not key study: Other studies (same reliability score) showing greater toxicity and with standard test organisms are available |

11.09.2003 (1) (8)

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

| | | |
|---|---|---|
| **Species** | : | Microcystis aeruginosa (Algae, blue, cyanobacteria) |
| **Endpoint** | : | biomass |
| **Exposure period** | : | 8 day(s) |
| **Unit** | : | mg/l |
| **Toxicity Threshold (TT)** | : | = 3.5 |
| **Limit test** | : | no |
| **Analytical monitoring** | : | no data |
| **Method** | : | other |
| **Year** | : | 1980 |
| **GLP** | : | no data |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Remark** | : | Tested in the cell multiplication inhibition test. The concentration of the algal suspension of each test culture was measured turbidimetrically and expressed as the extinction of the primary light of the monochromatic radiation at 578 nm for a 10 nm layer. Control cultures were monitored over the 8 day exposure period.<br>Toxicity threshold is the pollutant concentration causing the onset of cell multiplication inhibition. |
| **Result** | : | RESULTS: EXPOSED<br>TT = 3.5 mg/l<br>Based on measured results |
| **Source** | : | Bringman and Kuhn 1978. |
| **Test condition** | : | TEST ORGANISMS<br>Strain: Microcytis aeruginosa<br>Source/Supplier: Not reported<br>Pretreatment: None<br>Controls: 12 control cultures containing algal suspension, stock nutrient solution and bidistilled water under sterile conditions<br>STOCK AND TEST SOLUTION AND THEIR PREPARATION<br>Vehicle, solvent: Not reported<br>Concentration of vehicle, solvent: Not reported<br>STABILITY OF TEST CHEMICAL SOLUTIONS<br>Not reported<br>DILUTION WATER<br>Source: Standard algal medium<br>Aeration: Not reported<br>Alkalinity: Not reported<br>Hardness: Not reported<br>Conductance: Not reported |

TEST SYSTEM
Concentrations: Not reported
Renewal of test solution: Not reported
Exposure vessel type: Culture tubes stoppered with cotton-lined metal caps
Number of replicates: 3
Initial cell concentration: Quantity of cell material used for inoculation is determined turbidimetrically and is standardised.
Test temperature: 27 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: To neutral if required
Intensity of irradiation: Not reported
Photoperiod: Exposed to constant lighting by luminescent tubes (Osram L 40/30)2 in a central field between two lateral luminescent tubes at 60 cm distance from each other.
TEST PARAMETER: Growth
MONITORING OF TEST SUBSTANCE CONCENTRATION: Not reported

**Reliability** : (2) valid with restrictions
**Flag** : Critical study for SIDS endpoint
18.09.2003 (2)

**Species** : Scenedesmus quadricauda (Algae)
**Endpoint** : biomass
**Exposure period** : 8 day(s)
**Unit** : mg/l
**TT** : = 17
**Limit test** : no
**Analytical monitoring** : no data
**Method** : other
**Year** : 1978
**GLP** : no data
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Bringman and Kuhn 1978, Bringmann and Kuhn 1980.
**Reliability** : (2) valid with restrictions
Not key study: Other studies (same reliability scores) but with higher toxicity values are available.
18.09.2003 (2) (3)

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

**Type** :
**Species** : other protozoa: Entosiphon sulcatum
**Exposure period** : 72 hour(s)
**Unit** : mg/l
**TT or EC3** : = 31
**Analytical monitoring** : no data
**Method** : other
**Year** : 1980
**GLP** : no data
**Test substance** : other TS: Heptanol (111-70-6)

**Remark** : Dissolved toxic water ingredients will inhibit cell multiplication of the protozoan, Entosiphon sulcatum. Thus, in a test culture containing dissolved toxic substances the count of organisms, after a certain period will be less than in a test culture kept under identical conditions, however, free from toxic influence. The number of protozoa is determined by means of a cell counter.

**Source** : Bringmann and Kuhn 1980.
**Test condition** : TEST ORGANISMS
Strain: Entosiphon sulcatum
Supplier: Stock cultures
Feeding: Bacteria, Escherichia coli
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: Not reported
Vehicle, solvent: Not reported
Purity/supplier: Not reported
DILUTION WATER
Source: Not reported
Alkalinity: Not reported
Hardness: Not reported
Conductance: Not reported
TEST SYSTEM
Concentrations: Not reported
Dosing rate: Not reported
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 2
Test temperature: 25 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: None
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported
**Reliability** : (2) valid with restrictions
Best study although not a SIDS endpoint.

25.09.2003 (3)

**Type** : aquatic
**Species** : Pseudomonas putida (Bacteria)
**Exposure period** : 16 hour(s)
**Unit** : mg/l
**TT or EC3** : = 67
**Analytical monitoring** : no data
**Method** : other
**Year** : 1980
**GLP** : no data
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Bringmann and Kuhn 1980.
**Reliability** : (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

25.09.2003 (3)

**Type** :
**Species** : Uronema parduzci (Protozoa)
**Exposure period** :
**Unit** : mg/l
**EC0** : = 17
**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: Heptanol (111-70-6)

**Source** : Verschueren 1996.
**Reliability** : (4) not assignable
Not key study: Other studies with higher reliability score are available

01.10.2003 (12)

## 4.6.4 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

| | | |
|---|---|---|
| **Species** | : | other: Xenopus laevis (Clawed toad 3-4 weeks post-hatch) |
| **Endpoint** | : | |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | other: mg/l |
| **LC50** | : | = 44 |
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: Heptanol (111-70-6) |
| **Source** | : | Verschueren 1996. |
| **Reliability** | : | (4) not assignable |

30.10.2003 (12)

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**Method** :
**Year** :
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol

**Test condition** : These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including C6-C18 alcohols included in this category, form glucuronic acid conjugates in the rabbit.

Groups of 3 Chinchilla rabbits sex unspecified, about 3 kg in weight were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.

The results were reported as the amount of extra glucuronic acid excreted as a % of dose.

**Result** : The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:

n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.

No further information on other biotransformation pathways of these alcohols was provided.

**Conclusion** : All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose.

**Reliability** : (2) valid with restrictions

**Source** : Kamil, 1953
**Flag** : Critical study for SIDS endpoint
04.04.2005 (7) (10) (15)

**Method** :
**Year** :
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : Heptyl alcohol is oxidised to heptanoic acid which is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Reliability** : (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including n-heptanol.
05.04.2005 (14)

## 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | rat |
| **Strain** | : | Wistar |
| **Sex** | : | male/female |
| **Number of animals** | : | 120 |
| **Vehicle** | : | other: olive oil |
| **Value** | : | = 5500 - 6200 mg/kg bw |
| **Method** | : | other: in house protocol |
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ORGANISMS: rat
- Source: no data
- Age: young adults
- Weight at study initiation: mean weight males 250 g, females 200 g
- Group size: 10 male + 10 female
- Controls: no

ADMINISTRATION: gastric intubation
- Doses: 2500, 3500, 4100, 6150, 8200, 10250, 12300 mg/kg
- Doses per time period: single
- Volume administered or concentration: not reported
- Post dose observation period: 14 days

EXAMINATIONS: Clinical signs of intoxication, histopathological examination.

**Result** :

MORTALITY:
- Time of death: No animal died later than 6 days following ingestion the majority of deaths occurred within 48 hours.
- Number of deaths at each dose:
2500 mg/kg males and females 0/10
3500 mg/kg males and females 1/10
4100 mg/ke males 2/10; females 3/10
6150 mg/kg females only tested 6/10
8200 mg/kg males 3/10; females 7/10
10250 mg/kg males only tested 8/10
12300 mg/kg males 9/10; females 10/10

Male LD50 6200 mg/kg (+- 700)
Female LD50 5500 mg/kg (+- 500)

CLINICAL SIGNS: Rats which died showed symptoms of acute pulmonary oedema. In survivors recuperation was quite rapid.

NECROPSY FINDINGS: Irritation of the pulmonary epithelium with oedema and concestion, with macrophage infiltration. In females the congestion and inflammation were not dose related. In females dilation of the renal distal tubules was observed at high dose levels.

POTENTIAL TARGET ORGANS: Lung, kidney

**Remark** : Acute oral rat LD50 determined in this study is misreported in RTECS, 2004 as 500 mg/kg.

| | | |
|---|---|---|
| **Conclusion** | : | The rat oral LD50 for 1-heptanol was reported as 6200 mg/kg in males and 5500 mg/kg in females. Signs of intoxiciaton were typical of acute pulmonary oedema, this was confirmed by pahtological examination. Histopathological examinaiton revealed dilation of the kidney tubules in female rats. |
| **Reliability** | : | (2) valid with restrictions<br>Study well documented, meets generally accepted scientific principles, acceptable for assessment. |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | mouse |
| **Strain** | : | |
| **Sex** | : | male/female |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Value** | : | = 6000 mg/kg bw |
| **Method** | : | other |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test condition** | : | Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg for the series of alcohols tested). The actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination. n-heptanol was tested as part of a comparative study with other alcohols. |
| **Result** | : | The mouse LD50 value for n-heptanol is 6 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain. |
| **Reliability** | : | (4) not assignable<br>Original document in Russian (Zaeva, 1963, translation available), experimental detail insufficient to adequately assess validity. |

04.10.2004 (10) (11) (16)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | mouse |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Value** | : | = 4350 mg/kg bw |
| **Method** | : | |
| **Year** | : | 1982 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Secondary report of Russian original (unavailable). Mouse LD50 reported as 4350 mg/kg (+- 1650). No further details available. The value of 4.3 g/kg cited by Opdyke, 1975 and Patty 2001 is from the same source. |
| **Reliability** | : | (4) not assignable<br>Secondary reference to Russian data reported by Ismerov 1982. |

04.04.2005 (6) (10) (11) (12)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | rat |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Value** | : | = 3250 mg/kg bw |
| **Method** | : | |
| **Year** | : | 1960 |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Tertiary reports of unpublished data produced in the 1940's. |
| **Reliability** | : | (4) not assignable |

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| | | |
|---|---|---|
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | RTECS reports the following LD50 values obtained from Russian references which we do not have access to. These values have not been reported in Patty 2001 or in the Fragrance Raw Material Monograph for 1-heptanol, Opdyke 1975.<br><br>mouse oral LD50 1500 mg/kg, Russian literature report, 1966<br>rat oral LD50 3800 mg/kg, Russian reference text, 1984<br>rabbit oral LD50 750 mg/kg, Russian literature report, 1966 |
| **Reliability** | : | (4) not assignable<br>Secondary references to Russian literature sources , originals not available. |

04.04.2005 (12)

## 5.1.2 ACUTE INHALATION TOXICITY

| | | |
|---|---|---|
| **Type** | : | LC50 |
| **Species** | : | rat |
| **Strain** | : | Wistar |
| **Sex** | : | male/female |
| **Number of animals** | : | 20 |
| **Vehicle** | : | other: air |
| **Exposure time** | : | 4 hour(s) |
| **Method** | : | other |
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | TEST ANIMALS: rat<br>- Strain: Wistar<br>- Sex: male + female<br>- Source: not reported<br>- Age: young adults, |

- Weight: mean weights: males 250 g, females 200 g
- Number of animals: 10 males + 10 females
- Controls: no

ADMINISTRATION:
- Type of exposure: whole body inhalational exposure
- Concentrations: saturated vapour concentration
- Particle size: Not reported
- OBservation period: 15 days

EXAMINATIONS: clinical signs, histopathological examination of major organs.

**Result** : MORTALITY: None

CLINICAL SIGNS: None

NECROPSY FINDINGS: None

POTENTIAL TARGET ORGANS: None

SEX-SPECIFIC DIFFERENCES: None

**Conclusion** : The rat 4 hour LC50 for 1-heptanol is > saturated vapour concentration.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Flag** : Critical study for SIDS endpoint
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**Type** : LC50
**Species** : mouse
**Strain** :
**Sex** : no data
**Number of animals** :
**Vehicle** :
**Exposure time** :
**Value** : = 6.6 mg/l
**Method** :
**Year** : 1982
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : Secondary report of Russian literature original unobtainable. Mouse LC50 reported as 6.6 mg/l (+-2.9 mg/l). No further details available. RTECS, 2003 gives 3 literature citations for this value.

**Reliability** : (4) not assignable
Secondary references to Russian literature sources, original not available.
04.04.2005 (6) (10) (11) (12)

## 5.1.3 ACUTE DERMAL TOXICITY

**Type** : LD50
**Value** : ca. 2000 mg/kg bw
**Species** : rabbit
**Strain** : no data

| | | |
|---|---|---|
| **Sex** | : | no data |
| **Number of animals** | : | 18 |
| **Vehicle** | : | other: undiluted |
| **Doses** | : | 20.5, 32.8 and 41 g/kg (absorbed doses 0, 1.3 and 2.7 g/kg) |
| **Method** | : | other: modified Draize |
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ORGANISMS: rabbit
- Source: not reported
- Age: not reported
- Weight at study initiation:
- Group size: 6

ADMINISTRATION: dermal
- Area covered: 250 -400 cm2 (this included the ventral surface as well as the back and flanks all of which were shaved)
- Occlusion: no data
- Vehicle: undiluted
- Total volume applied: 25-50 ml
- Doses: 20.5, 32.8 and 41 g/kg
- Removal of test substance: no data
- Observation period: Some test aniamsl were sacrificed 2 weeks after exposure the remainder after 6 weeks.

EXAMINATIONS: clinical signs, gross and microscopic pathological examination.

**Result** :

MORTALITY:
- Time of death:
- Number of deaths at each dose:
20.5 g/kg 0/6
32.8 g/kg 2/6
41.0 g/kg 4/6

APPLICATION SITE: Lesions comparable to chemical burns.

CLINICAL SIGNS: At the higher dose levels there was up to 40% reduction in body weight over the observation period in spite of normal food consumption. Some surviving animals were sacrificed at 2 weeks others at 6 weeks.

NECROPSY FINDINGS: no changes in the major organs (lungs, heart, liver, pancreas, kidneys, testes. All animals examined showed the following changes in the brain: spongiform appearance of the glial tissue particularly in the grey matter more noticeable 6 weeks after treatment, also perivascular oedema. One control animal also showed similar lesions.

POTENTIAL TARGET ORGANS: brain

**Conclusion** : The approximate rabbit dermal LD50 is reported by the authors as ca 2 g/kg (absorbed dose). The actual dose administered was up to 50 ml/kg. Severe skin irritation was observed at the application site.

**Reliability** : (3) invalid
In view of the very large doses applied to a major portion of the skin of these animals and the degree of irritation (described as chemical burns) the results of this study are not considered valid. No indication was given

as to how the so-called absorbed dose was determined. The value is also reported in secondary references.

**Source** : Truhaut, 1974

**Flag** : Critical study for SIDS endpoint
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**Type** : LD50
**Value** : > 5000 mg/kg bw
**Species** : rabbit
**Strain** :
**Sex** : no data
**Number of animals** :
**Vehicle** : no data
**Doses** :
**Method** : other
**Year** : 1974
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Reliability** : (4) not assignable
Secondary reference to unpublished data provided by Moreno, 1974

**Source** : Opdyke, 1975

**Flag** : Critical study for SIDS endpoint
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## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

**Species** : rabbit
**Concentration** : undiluted
**Exposure** : no data
**Exposure time** : no data
**Number of animals** : 6
**PDII** : .5
**Result** : slightly irritating
**EC classification** : not irritating
**Method** : other: modified Draize Test
**Year** : 1974
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ANIMALS: rabbits
- Number of animals: 6

ADMINISTRATION/EXPOSURE
- Preparation of test substance: undiluted
- Area of exposure: no data
- Occlusion: no data
- Vehicle: undiluted
- Total volume applied: 0.5 ml
- Postexposure period: 72 hours

- Removal of test substance: no data

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 24 and 72 hours

**Result** : AVERAGE SCORE mean 24+48 hours intact and scarified
- Erythema: 0 (intact skin); 0.75 (abraded skin)
- Oedema: 0 (intact skin); 0.25 (abraded skin)

Maximum score 1

PII 0.5

REVERSIBILITY: At the abraded sites irritation was still evident in some rabbits at 72 hours although the incidence was reduced. For erythema 6/6 scored 1 at 24 hours and 3/6 at 72 hours, for oedema 2/6 scored 1 at 24 hours 1/6 at 72 hours.

OTHER EFFECTS: None reported

**Conclusion** : 1-heptanol is not irritating to the skin according to either EU or GHS criteria.

**Reliability** : (2) valid with restrictions
Test in accordance with national standard methods with acceptable restrictions. Incomplete documentation of method but results given in full, observation period limited to 72 hours but indication of reversal of effect.

**Flag** : Critical study for SIDS endpoint
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**Species** : rabbit
**Concentration** : undiluted
**Exposure** : Occlusive
**Exposure time** : 6 day(s)
**Number of animals** : 5
**PDII** :
**Result** : highly irritating
**EC classification** :
**Method** : other: repeated skin application
**Year** : 1963
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

**Test condition** : Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental details were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol.

**Result** : The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol.

| | | |
|---|---|---|
| **Conclusion** | : | Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit skin for 6 consecutive days resulted in marked irritation with eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol. |
| **Reliability** | : | (4) not assignable<br>Non standard test with limited documentation. |
| **Source** | : | Zaeva, 1963 |

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| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Exposure** | : | Occlusive |
| **Exposure time** | : | 24 hour(s) |
| **Number of animals** | : | |
| **PDII** | : | |
| **Result** | : | moderately irritating |
| **EC classification** | : | |
| **Method** | : | Draize Test |
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Following 24 hour occlusive application of the undiluted material to intact and abraded skin 1-heptanol was described as a moderate irritant. This is a secondary report of unpublished data (Moreno, 1974) and no further information is available. |
| **Reliability** | : | (4) not assignable<br>Secondary reference. |
| **Source** | : | Opdyke, 1975 |

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| | | |
|---|---|---|
| **Species** | : | human |
| **Concentration** | : | 1 % |
| **Exposure** | : | Occlusive |
| **Exposure time** | : | 48 hour(s) |
| **Number of animals** | : | |
| **PDII** | : | |
| **Result** | : | not irritating |
| **EC classification** | : | |
| **Method** | : | other |
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Secondary report of unpublished data from (Epstein, 1974). When tested in a 48 hour closed patch test in human volunteers at a concentration of 1% in petrolatum there was no evidence of skin irritation. No other experimental details available. |
| **Reliability** | : | (4) not assignable<br>Secondary reference. |
| **Source** | : | Opdyke, 1975 |

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## 5.2.2 EYE IRRITATION

| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Dose** | : | .1 ml |
| **Exposure Time** | : | |
| **Comment** | : | not rinsed |
| **Number of animals** | : | 6 |
| **Result** | : | moderately irritating |
| **EC classification** | : | |
| **Method** | : | Draize Test |
| **Year** | : | 1959 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ANIMALS: Rabbit
- Sex: No data
- Source: No data
- Age: No data
- Weight at study initiation: No data
- Number of animals: 6
- Controls: the other eye

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted
- Amount of substance instilled: 0.1 ml
- Postexposure period: 7 days

EXAMINATIONS
- Scoring system: Draize plus Kay and Calandra.
- Observation period: 7 days
- Tool used to assess score: Not reported

**Result** :

AVERAGE SCORE (24+48+72 hour mean scores)
- Cornea: 1.12 (max score 3)
- Iris: 0
- Conjunctivae (Redness): 0.9 (max score 2)
- Conjunctivae (Chemosis): 0.2 (max score 1)

Individual 24+48+72 hour mean scores for corneal opacity are 2, 0.3, 1, 1, 0.8, 1.

REVERSIBILITY:
Group mean scores at 94 hours
- Cornea: 1.5 (max score 3)
- Iris: 0
- Conjunctivae (Redness): 0.3 (max score 1)
- Conjunctivae (Chemosis): 0

Group mean scores at 7 days
- Cornea: 0.5 (max score 2)
- Iris: 0
- Conjunctivae (Redness): 0.12 (max score 1)
- Conjunctivae (Chemosis): 0

The study was terminated at 7 dyas by which time there was evidence of regression of the lesions in all animals.

| | | |
|---|---|---|
| **Conclusion** | : | 1-heptanol is not classifiable as a skin irritant according to EU criteria but would be classified as a Class 2A irritant according to GHS criteria. This is based on individual mean 24+48+72 hour scores of >= 1 for corneal opacity in 4/6 animals tested and persistence to 7 days of some corneal opacity in 2 animals. |
| **Reliability** | : | (2) valid with restrictions<br>Test procedure in accordance with National standard methods with acceptable restrictions. |
| **Source** | : | Truhaut, 1974 |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Species** | : | rat |
| **Concentration** | : | undiluted |
| **Dose** | : | other: one drop |
| **Exposure Time** | : | |
| **Comment** | : | |
| **Number of animals** | : | 5 |
| **Result** | : | corrosive |
| **EC classification** | : | |
| **Method** | : | other: non standard |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | The following alcohols were investigated in this comparative study: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol |
| **Test condition** | : | One drop of undiluted material was instilled into the eye of 5 rabbits. No further experimental details are reported. |
| **Result** | : | All the alcohols studied caused redness and swelling of the mucous membranes of the eye. These disappeared almost completely within 4-5 hours. The most marked changes were observed with n-hexanol and are described as suppurative conjunctivitis and cloudiness of the cornea. There is no information given on the reversibility of these changes. The results suggest that except for 1-hexanol the alcohols tested are at most slightly irritating to the eye. |
| **Reliability** | : | (3) invalid<br>Documentation insufficient for assessment. |
| **Source** | : | Zaeva, 1963 |

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## 5.3 SENSITIZATION

| | | |
|---|---|---|
| **Type** | : | other: human maximisation test |
| **Species** | : | human |
| **Concentration** | : | |
| | | Challenge 1 % |
| **Number of animals** | : | 20 |
| **Vehicle** | : | petrolatum |
| **Result** | : | not sensitizing |
| **Classification** | : | |
| **Method** | : | other: Magnusson & Kligman |

| | | |
|---|---|---|
| **Year** | : | 1974 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | 20 human volunteers were tested using 1% 1-heptanol in petrolatum in a maximisation test. No further details reported in this secondary reference (Epstein, 1974). |
| **Reliability** | : | (4) not assignable<br>Secondary reference. |
| **Flag** | : | Critical study for SIDS endpoint |

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## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | no data |
| **Strain** | : | |
| **Route of admin.** | : | inhalation |
| **Exposure period** | : | 4.5 months, 2 hours/day |
| **Frequency of treatment** | : | 6 days/week |
| **Post obs. period** | : | none |
| **Doses** | : | Single exposure level between 0.18 and 0.35 mg/l |
| **Control group** | : | yes, concurrent no treatment |
| **Method** | : | other |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test condition** | : | Groups of 8 rats were exposed to a single dose level of either n-heptyl, n-octyl (2-octanol) or n-decyl alcohol for 2 hours/day, 6 days/week for 4.5 months. The actual dose level at which each alcohol was tested was not reported, the dose levels were reported as between 0.18 and 0.35 mg/l (33.8 - 56.3 ppm). There was a concurrent control group consisting of 8 untreated animals. The effect of these alcohols on the test animals was evaluated by clinical observations, body weight gain, neuromuscular response to electrical stimulation, effect on peripheral blood [Hb, RBC, WBC (plus differential WBC count)] together with macroscopic and histopathological examination of some organs. |
| **Result** | : | Minor changes in haematological parameters (decreased Hb & white cell count) were not of statistical significance. A reversible increase in the threshold of neuromuscular excitability was observed after 3.5 months exposure to n-heptanol(9.6(+-0.26) mA and 2-octanol 9.2(+-0.35 mA) compared to controls 8.2(+-0.25 mA). The behaviour of the exposed animals was comparable to that of controls as was body weight gain. There were no gross pathological changes. Minor histopathological changes (dystrophic) were reported in various organs including the liver, kidneys and myocardium. The incidence of these changes in treated and control animals was not clearly reported, the effects appeared more marked in animals exposed to n-heptanol and 2-octanol. With n-heptanol and 2-octanol there was some evidence of mild irritation of the respiratory tract.<br><br>Also reported briefly by Opdyke, 1975 |
| **Reliability** | : | (3) invalid<br>Significant methodological deficiences and insufficient documentation for |

assessment.

**Source** : Zaeva, 1963
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**Remark** : Summary data of Russian studies reported by RTECS and/or Patty 2001 as follows:

Mammalian (species unspecified) inhalation exposure. Lowest published toxic concentration reported as 180 mg/m3/2 hour/137 day-intermittent. Unspecified changes in the respiratory system, liver and urinary system. (RTECS)

Mammalian (species unspecified) inhalation exposure. Lowest published toxic concentration reported as 32 mg/m3/26 week intermittent. Effects reported on the optic nerve together with other unspecified effects on the eye. (RTECS)

Rabbit, oral. Lowest published toxic dose 4.56 mg/kg/day for 26 weeks, intermittent. An effect on cholinesterase reported. (RTECS, Patty, Opdyke)

**Reliability** : (4) not assignable
Secondry references original unobtainable.
05.04.2005 (10) (11) (12)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : other
**System of testing** : Chinese hamster V79 cells
**Concentration** : 2 mmoles/l
**Cycotoxic conc.** :
**Metabolic activation** :
**Result** :
**Method** : other
**Year** : 1987
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : In this investigative study to determine markers for aneugenicity, 10(6) Chinese hamster lung cells (V79) were seeded for measurements of cell survival, aneuploidy and c-mitotic activity and cultured for 20-24 hours prior to treatment with the test substance. Incubation with the test substance (conc. 2 mmoles/l) was for 30 minutes (c-mitosis, survival) or 3 hours (aneuploidy). Following treatment the slides were fixed, dried and stained. Normal and affected metaphases, anaphases and iclophases were scored for c-mitosis (100 mitotic cells/slide, 2 slides per dose for each experiment). Only those metaphases (100-200/slide) with 21 or more chromosomes were scored for aneuploidy. Because of the low solubility acetone was used to produce the test concentration.

**Result** : Survival was 68% in the test cultures at 30 minutes. The number of cells with >22 chromosomes after 3 hours exposure to 2mmoles/l 1-heptanol was 11.6% in the test group [12/103] compared to 25/500 and 29/592 in the control groups, 5 and 4.9 % respectively. The significance of this increase was $p < 0.025$. As cell survival decreased, c-mitosis increased. Based on the dose response observed for the induction of c-mitosis and aneugenicity and together with the cytotoxicity profile the authors

concluded that the effect on spindle function of highly lipophilic compounds including 1-heptanol was most likely induced through an indirect (physical) mechanism relating to the partitioning of the test substance into cellular hydrophobic compartments and not related to a direct interaction with spindle formation and function.

**Conclusion** : This investigative study into markers for potential aneugenicity showed that 1-heptanol caused increased aneuploidy and C mitosis. The study authors noted that for the aliphatic alcohols the threshold for the aneugenic responses and the cytotoxicity were very close and concluded that the observed effects reflected physico-chemical interactions rather than a true indication of potential genotoxicity

**Reliability** : (3) invalid
There is no information presented to verify that adequate quality assurance methods were in place to ensure that the test system functioned appropriately. Presently, in-vitro assays to detect aneuploidy rely on more sensitive, alternative methods and the validity of the data presented in this study are therefore uncertain (ECETOC Monograph 27, Aneuploidy, 1997).

**Source** : Onfelt, 1987
29.12.2005 (9) (12)

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Cytogenetic assay
**Species** : rat
**Sex** : male
**Strain** :
**Route of admin.** : other: intragastric
**Exposure period** : 48 hours
**Doses** : 1/5th LD50
**Result** : ambiguous
**Method** : other
**Year** : 1988
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage
- Vehicle: Homogenised emulsion
- Duration of test: 48 hours
- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were

reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Result** : MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:

600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 2.4 +-0.7
Cells with breakages %: controls 0.3 +-0.2; treated 1.0 +-0.4; Cells with chromosome aberrations %: controls 0; treated 2.2 +-0.6.

STATISTICAL RESULTS: Reported as above.

**Conclusion** : Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability** : (3) invalid
Significant methodological deficiencies (see test conditions).

**Source** : Barilyak, 1988
08.10.2004 (1)

## 5.7 CARCINOGENITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

## 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

**Type** : other: Aspiration

**Remark** : Aspiration of 0.2 ml 1-heptanol to rats produced immediate death in 10/10 rats following respiratory arrest.

**Reliability** : (2) valid with restrictions

04.10.2004 (3)

**Type** : other: Sensory irritation

**Remark** : The RD50 for n-hexanol was reported as 100 ppm in Swiss mice. Exposure time not reported. The original paper (Muller & Greff, 1984) reports unpublished data which is summarised in Bos et al, 1992.

**Reliability** : (4) not assignable
Secondary report.

04.10.2004 (2) (8)

**Type** : other: Sensory irritation

**Remark** : Groups of 4 CF1 mice were exposed head only to various alcohols including 1-heptanol. Sensory irritation, pulmonary irritation and anaesthesia were evaluated. Anaesthesia was not observed with 1-heptanol concentrations up to 10100 ppm. the RD50 (0-10 mins) was found to be 700 ppm. Pulmonary irritation did not interfere with the sensory irritation response of 1-heptanol.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

04.10.2004 (4)

**REFERENCES FOR PHYS CHEM, ENVIRONMENTAL FATE AND ECOTOXICITY PARTS**

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**REFERENCES FOR HUMAN HEALTH ENDPOINTS**

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(2) Bos, P.M.J et al 1992 Evaluation of the sensory irritation test for the assessment of occupational health risk. Critical Reviews in Toxicol. 21(6):423-450

(3) Gerarde, H.W.; Ahlstrom, D.B. 1966 The aspiration hazard and toxicity of a homologous series of alcohols. Arch. Env. Hlth. 13:457-461

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(6) Ismerov, N.F. et al 1982 Toxicometric parameters of industrial toxic chemicals under single exposure. USSR/UNEP-IRPTC Publication, 1982

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# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

Note: References in this file are given separately for physicochemical properties, environmental fate, ecotoxicology (i.e. chapters 2-4) and human health endpoints (chapter 5).

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 143-08-8 |
| **CAS No.** | **:** | 143-08-8 |
| **EINECS Name** | **:** | nonan-1-ol |
| **EC No.** | **:** | 205-583-7 |
| **Molecular Formula** | **:** | C9H20O |

## 2.1 Melting Point

**Value:** = -5 degree C

**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (14)

## 2.2 Boiling Point

**Value:** = 194 - 213 degree C

**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (14)

## 2.3 Density

**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (14)

## 2.4 Vapour Pressure

**Value:** = .0133 hPa at 25 degree C

**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Clayton and Clayton 1994.
**Reliability:** (4) not assignable
30-SEP-2003 (4)

**Value:** = .03 hPa at 25 degree C

**Method:** other (measured)
**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Daubert and Danner 1989.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (5)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water

**log Pow:** = 3.77

**Method:** other (measured)
**Test substance:** other TS: Nonanol (143-08-8)

**Method:** The generator column was coated with liquid solute and 1-octanol. Water was then pumped into the column. Analysis of the aqueous phase from the 1% octanol coated column was used to determine the Kow.
**Source:** Tewari et al. 1982.
**Reliability:** (2) valid with restrictions
24-SEP-2003 (10)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 128 mg/l at 20 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Letinski 2002.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (7)

**Solubility in:** Water
**Value:** = 1000 mg/l at 20 degree C

**Method:** other
**Test substance:** other TS: Nonanol (143-08-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
29-OCT-2003 (14)

**Solubility in:** Water
**Value:** = 140 mg/l at 25 degree C

**Method:** other (measured)
**Test substance:** other TS: Nonanol (143-08-8)

**Source:** SRC.
**Reliability:** (4) not assignable
29-OCT-2003 (9)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**GLP:** no data
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.
**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.
**Result:** 47.9% degradation after 5 days (% ThOD)
**Source:** Vaishnav et al. 1987.
**Test substance:** Nonanol (143-08-8)
**Reliability:** (2) valid with restrictions
13-AUG-2003 (11)

# AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 5.52
**Limit Test:** no

**Method:** other: ASTM 1980
**Year:** 1985
**GLP:** no data
**Test substance:** other TS: Nonanol (143-08-8)

**Remark:** Flow-through toxicity tests were conducted with a geometric series (0.8 dilution factor) of toxicant concentrations for all tests. Test water was maintained at 25 C and pH 7.6. Five fry or juveniles were added to each treatment and control chamber, providing a total of 20 test organisms per treatment level.
The test was performed in 1985.

**Result:** RESULTS: EXPOSED
LC50 = 5.52 mg/l for fry
Based on measured concentrations
RESULTS: CONTROL
Number/% showing adverse effects: not reported

**Source:** Broderius et al. 1985.

**Test condition:** TEST ORGANISMS
Strain: Fathead minnow
Supplier: Not reported
Age: Newly hatched fry were < 24 hours old
Weight: Not reported
Feeding: Spawning stock and juveniles were cultured on recently hatched brine shrimp nauplii (Artemia sp.) and frozen adult brine shrimp
Pretreatment: Acclimated to test chambers for 2-3 hours prior to introduction of toxicants
Feeding during test: none
Control group: 1 control group (5 fish)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle: not reported
Concentration of vehicle/solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: Aeration in head water reservoirs
Alkalinity: 44.0 mg/L as CaCO3
Hardness: 44.6 mg/l
Conductance: not reported
TEST SYSTEM
Concentrations: not reported but publication indicates daily analytical monitoring was conducted
Renewal of test solution: water replacement 2-4 h (25mL/min)
Exposure vessel type: Glass with silicone sealant
Number of replicates: 4
Fish per replicate: 5

Test temperature: mean 25C
Dissolved oxygen: above 80% saturation
pH mean: 7.6
Adjustment of pH: not reported
Intensity of irradiation: 22 to 38 lumens/sq ft
Photoperiod: Illuminated with wide spectrum fluorescent bulbs for 16 h daily
TEST PARAMETER: lethality
SAMPLING: mortalities recorded daily
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
11-SEP-2003 (2)

**Type:** static
**Species:** Alburnus alburnus (Fish, estuary)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50:** = 18
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** other TS: Nonanol (143-08-8)

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Ten fish were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Source:** Bengtsson, 1984
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with greater toxicity are available
19-AUG-2003 (1) (8)

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 5.7
**Limit Test:** no

**Method:** other: USEPA 1975
**Year:** 1983
**GLP:** no data
**Test substance:** other TS: Nonanol (143-08-8)

**Method:** Twenty to twenty five 30-day old fish were randomly divided among twelve test tanks (a control and five different concentrations, in duplicate). Fish not fed during the test.
**Source:** Veith et al. 1983a; Veith et al. 1983b; Brooke et al. 1984.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

11-SEP-2003 (3) (12) (13)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 25
**Limit Test:** no

**Method:** other:
**Year:** 1979
**GLP:** no data
**Test substance:** other TS: Nonanol (143-08-8)

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Result:** RESULTS: EXPOSED
LC50 = 25 mg/l
based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
**Source:** Bengtsson, 1984
**Test condition:** TEST ORGANISMS
Strain: Nitocra spinipes
Supplier: Laboratory culture
Weight: not reported
Feeding: not reported
Pretreatment: not reported
Feeding during test: not fed during test
Control group: 2 control group (10 individuals in each)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle, solvent: concentration never exceeded 500 ul/l
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Natural Brackish water (filtered before use)
Aeration: No aeration
Alkalinity: 1.6 megv/l
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: Logarithmic series of at least 6 concentrations
Renewal of test solution: none
Exposure vessel type: 15ml standard laboratory test tubes
Number of replicates: 2

Invertebrate per replicate: 10

Test temperature: 21 +/- 1 C
Dissolved oxygen: Not reported
pH mean: 7.9
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported
TEST PARAMETER: lethality
SAMPLING: Mortality was recorded only after 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION:
not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
12-MAR-2004 (1) (8)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 100

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** other TS: Nonanol (143-08-8)

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
**Source:** Hattori 1987.
**Reliability:** (3) invalid
Best study although not a SIDS endpoint.
Study was considered invalid due to significant methodological deficiencies.
25-SEP-2003 (6)

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**Test substance** : n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol

**Test condition** : These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including C6-C18 alcohols included in this category, form glucuronic acid conjugates in the rabbit.

Groups of 3 Chinchilla rabbits, about 3 kg in weight, were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.

The results were reported as the amount of extra glucuronic acid excreted as a % of dose.

**Result** : The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:

n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.

No further information on other biotransformation pathways of these alcohols was provided.

**Conclusion** : All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose.

**Reliability** : (2) valid with restrictions
Publication, reasonable documentation, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Kamil et al, 1953
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
05.04.2005 (6)

**Remark** : 1-nonanol is oxidised to nonanal which is rapidly oxidised to nonanoic acid. Nonanoic acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Reliability** : (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including 1-nonanol.
25.11.2004 (12)

## 5.1.1 ACUTE ORAL TOXICITY

**Type** : LD50
**Species** : mouse

| | | |
|---|---|---|
| **Strain** | : | no data |
| **Sex** | : | no data |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Value** | : | = 20000 mg/kg bw |
| **Method** | : | other |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test condition** | : | Groups of 6 mice received the test material undiluted at various dose levels (these ranged between 1 and 35 g/kg for the series of alcohols tested). The actual dose levels were not reported. The animals were observed for 14 days after dosing and the animals which died were subject to pathological examination. 1-nonanol was tested as part of a comparative study with other alcohols. |
| **Result** | : | The mouse LD50 value for n-heptanol is 20 g/kg. The minimum lethal dose was 10 g/kg. Signs of intoxication were lack of coordination, respiratory distress, hyperactivity and convulsive twitching. Pathological examination of mice which died revealed hyperaemia of the internal organs and brain.<br><br>Cited in RTECS, 2004 |
| **Reliability** | : | (4) not assignable<br>Original document in Russian (Zaeva, 1963, translation available), experimental detail insufficient to adequately assess validity. |
| **Source** | : | Zaeva, 1963 |

07.04.2005 (11) (13)

| | | |
|---|---|---|
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: nonyl aclohol containing 2% 2-propyl heptanol |
| **Remark** | : | The rat and mouse LD50's for this sample of nonyl alcohol containing 2% 2-propyl heptanol are 3.2 - 6.4 g/kg and 6.4 - 12.8 g/kg respectively. No other details are available. The data were obtained from a personal communication ex D. Fassett originally reported in Patty 2nd revised edition, 1963. Compositional detail added in Patty 2001.<br><br>Cited in RTECS, 2004 |
| **Reliability** | : | (4) not assignable<br>Secondary reference. |

07.04.2005 (9) (10) (11)

### 5.1.2 ACUTE INHALATION TOXICITY

| | | |
|---|---|---|
| **Method** | : | |
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | other TS: nonyl aclohol containing 2% 2-propyl heptanol |
| **Remark** | : | The rat inhalational LC50 for this sample of nonyl alcohol containing 2% 2-propyl heptanol is >730 ppm for a 6 hour exposure. There were no deaths, no other experimental details are available. The data were obtained from a personal communication ex D. Fassett originally reported in Patty 2nd revised edition, 1963. Compositional detail added in Patty 2001. |

**Reliability** : (4) not assignable
Secondary reference.
15.09.2004 (10)

**Method** :
**Year** :
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : The acute inhalational LD50 in mice is reported as 5.5 mg/l, following a 2 hour exposure. This is a secondary reference to a Russian study reported in abstract only.

**Reliability** : (4) not assignable
Secondary reports of unobtainable Russian reference.
07.04.2005 (4) (10) (11)

### 5.1.3 ACUTE DERMAL TOXICITY

**Method** :
**Year** :
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : The acute dermal LD50 in rabbits is reported as 2.96 g/kg. This is a secondary reference to a Russian study reported in abstract only.

**Reliability** : (4) not assignable
Secondary reference.
15.09.2004 (10)

**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: nonyl aclohol containing 2% 2-propyl heptanol

**Remark** : The rabbit dermal LD50 for this sample of nonyl alcohol containing 2% 2-propyl heptanol is >10 ml/kg. No other details are available. The data were obtained from a personal communication ex D. Fassett originally reported in Patty 2nd revised edition, 1963. Compositional detail added in Patty 2001.

**Reliability** : (4) not assignable
Secondary reference.
15.09.2004 (10)

**Method** :
**Year** :
**GLP** :
**Test substance** : other TS: diisobutyl carbinol

**Remark** : The rabbit 24 hour dermal LD50 value of 5.66 ml/kg reported for n-nonyl alcohol by Opdyke is actually a value for the isomer diisbutyl carbinol originally reported in Patty 1963 (2nd revised edition). Also cited by RTECS.

**Reliability** : (4) not assignable
Secondary reference.

07.04.2005 (9)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

**Remark** : Not required OECD or HPV endpoint.
**Source** : The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07.03.2000

### 5.2.1 SKIN IRRITATION

**Species** : rabbit
**Concentration** :
**Exposure** : Occlusive
**Exposure time** : 4 hour(s)
**Number of animals** : 6
**PDII** :
**Result** : irritating
**EC classification** : irritating
**Method** : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year** : 1992
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Number of animals: 6

ADMINISTRATION/EXPOSURE
- Preparation of test substance: Undiluted or in polyethylene glycol 400 (PEG400)
- Area of exposure: 6x6 cm
- Occlusion: Under exposure chamber of 6X6 cm
- Conc. in vehicle: Undiluted or 50% in PEG.
- Exposure period: 4 hours
- Postexposure period: 72 hours
- Removal of test substance: Not reported
- Controls: The skin irritancy of PEG400 was not reported.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours.

**Result** : AVERAGE SCORE (individual animal scores were not reported)
Undiluted
- Erythema: Group mean 24+48+72 hour score 2.2
- Edema: Group mean 24+48+72 hour score 0

50% nonanol in PEG400
- Erythema: Group mean 24+48+72 hour score 1.9
- Edema: Group mean 24+48+72 hour score 0.2

REVERSIBILITY: Erythema had not reduced by the end of the 72 hour

exposure period.

| | | |
|---|---|---|
| **Conclusion** | : | Following 4 hour occlusive application to rabbit skin undiluted 1-nonanol can be considered as irritant under EU and GHS criteria based on mean scores >= 2 (EU) and persistence or the irritant response throughout the 72 hour observation period. |
| **Reliability** | : | (2) valid with restrictions<br>Guideline study without detailed documentation. |
| **Source** | : | Jacobs & Martens, 1992a<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |
| 10.08.2005 | | (5) |

| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | 100 % |
| **Exposure** | : | Occlusive |
| **Exposure time** | : | 6 day(s) |
| **Number of animals** | : | 5 |
| **PDII** | : | |
| **Result** | : | highly irritating |
| **EC classification** | : | |
| **Method** | : | other: repeated skin application |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol |
| **Test condition** | : | Groups of 5 rabbits received a daily topical application of 2 ml undiluted alcohol to the shorn skin for 6 days, no further experimental detaols were available. No individual scores were reported. Four primary alcohols were tested n-hexanol, n-heptanol, n-nonanol and n-decanol. Also tested was the secondary alcohol 2-octanol. |
| **Result** | : | The development of the irritative response was similar for all of the alcohols tested. There was a slight reddening of the skin on the initial days following application which developed by days 5-6 to marked redness and inflammation of the skin with the formation of deep cracks. The skin healed witin 10-12 days with the formation of numerous scabs, followed by exfoliation and marked skin pigmentation. Irritation was most marked with n-hexanol and 2-octanol and least marked with n-decanol. |
| **Conclusion** | : | Repeated application of C6, 7, 8, 9 and 10 alcohols to rabbit skin for 6 consecutive days resulted in marked irritation with eschar. The most marked irritation was seen with n-hexanol and 2-octanol, the least irritation was observed with n-decanol. |
| **Reliability** | : | (4) not assignable<br>Non-standard test with limited documentation. |
| **Source** | : | Zaeva, 1963 |
| 07.04.2005 | | (13) |

| | | |
|---|---|---|
| **Test substance** | : | Reported as 1-nonanol no other details given. |
| **Remark** | : | Secondary report indicating that 2% petrolatum applied to the skin of 25 human volunteers did not produce skin irritation. (Kligman, 1972 unpublished) No further experimental details available. |
| **Reliability** | : | (4) not assignable |

Secondary reference.

**Source** : Opdyke, 1973

06.04.2005 (9) (10)

### 5.2.2 EYE IRRITATION

| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Dose** | : | other: one drop |
| **Exposure Time** | : | |
| **Comment** | : | |
| **Number of animals** | : | 5 |
| **Result** | : | |
| **EC classification** | : | |
| **Method** | : | other: non standard |
| **Year** | : | 1963 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : The following alcohols were investigated in this comparative study: 1-hexanol, 2-octanol, 1-heptanol, n-nonanol, n-decanol

**Test condition** : One drop of undiluted material was instilled into the eye of 5 rabbits. No further experimental details are reported.

**Result** : All the alcohols studied caused redness and swelling of the mucous membranes of the eye. These disappeared almost completely within 4-5 hours. The most marked changes were observed with n-hexanol and are described as suppurative conjunctivitis and cloudiness of the cornea. There is no information given on the reversibility of these changes. The results suggest that except for 1-hexanol the alcohols tested are at most slightly irritating to the eye.

**Reliability** : (3) invalid
Documentation insufficient for assessment.

15.09.2004 (13)

**Remark** : Patty reports an eye irritation study by Jacobs & Martens, 1987, however this reference was to a skin irritation test.

07.04.2005 (10)

### 5.3 SENSITIZATION

| | | |
|---|---|---|
| **Type** | : | other: maximization test |
| **Species** | : | human |
| **Number of animals** | : | 25 |
| **Vehicle** | : | petrolatum |
| **Result** | : | not sensitizing |
| **Classification** | : | not sensitizing |
| **Method** | : | other: Kligman human maximization test |
| **Year** | : | 1973 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** : This patch test was carried out using the maximization procedure described by Kligman, A.M.the identification of contact allergens by human assay. III The maximization test: A procedure for screening and rating

contact allergens. J. Invest. Dermatol. 47:393-409, 1966. There are variations in this procedure but we have no information as to which variation was used. The exposure would have been a 48 hour occlusive exposure and sodium lauryl sulphate may have been used to promote the response. The only experimental detail given for 1-nonanol was that a panel of 25 volunteers were tested at a concentration of 2% in petrolatum. There is no indication as to whether this was an induction or challenge concentration.

**Result** : Under the conditions of this test 1-nonanol was not a human skin sensitiser.

**Remark** : This reference gives a summary report of unpublished data provided by Kligman 1972.

**Reliability** : (4) not assignable
**Source** : Opdyke, 1973
Hayes Consultancy Service Bromley, Kent

15.09.2004 (9) (10)

## 5.4 REPEATED DOSE TOXICITY

## 5.5 GENETIC TOXICITY 'IN VITRO'

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Cytogenetic assay
**Species** : rat
**Sex** : male
**Strain** :
**Route of admin.** : other: intragastric
**Exposure period** : 48 hour(s)
**Doses** : 1/5th LD50
**Result** : ambiguous
**Method** : other: non standard
**Year** : 1988
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS: Rats (outbred, strain not reported)
- Age: Not reported
- Weight at study initiation: 150-170g
- No. of animals per dose: 8 males/group

ADMINISTRATION: Gavage
- Vehicle: Homogenised emulsion
- Duration of test: 48 hours
- Frequency of treatment: Single dose
- Sampling times and number of samples: 48 hours
- Control groups and treatment: 10 males received 1 ml distilled water each.

EXAMINATIONS:
- Clinical observations: None reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Statistical difference between treated and

control parameters using analysis of variance.
- Criteria for selection of M.T.D.: Single dose selected as 1/5th LD50 as obtained from an earlier (1976) Russian publication. The actual LD50 was not given in the report. LD50's for the series of alcohols tested were reportedly between 2.26 and 12.8 mg/kg. (mg/kg may be a misprint in the original as more recent values for the acute oral LD50 are of the order of 4000 mg/kg).

DEVIATIONS FROM GUIDELINE PROTOCOL:
One sex used, no clinical examinations reported.
Insufficient information to indicate whether the single dose adminstered was the MTD or high enough to be considered as a limit dose.
No positive control group
No use of spindle inhibitor to arrest cell division at metaphase, cells in metaphase were selected for examination.
No measurement of the mitotic index.
It is not clear how many cells/animal were analysed (results appear to refer to total numbers of cells analysed/group).
No individual animal data, different types of chromosome aberrations not reported.

**Result** : MORTALITY: None reported

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: Not carried out

BODY WEIGHT CHANGES: No data

FOOD AND WATER CONSUMPTION CHANGES: No data

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: Not carried out

MUTANT/ABERRATION/mPCE/ POLYPLOIDY FREQUENCY:

600 control cells and 500 treated cells were analysed.
Polyploid cells %: controls 0.5 +-0.3; treated 0.2 +-0.2
Cells with breakages %: controls 0.3 +-0.2; treated 1.4 +-0.5; Cells with chromosome aberrations %: controls 0; treated 3.0 +-0.8.

STATISTICAL RESULTS: Reported as above.

**Conclusion** : Although the data presented suggest an increase in % of polyploid cells and cells with chromosome aberrations significant methodological deficiences render this study invalid.

**Reliability** : (3) invalid
Significant methodological deficiences (see test conditions).

**Source** : Barilyak, 1988
08.10.2004 (2)

## 5.7 CARCINOGENITY

## 5.8.1 TOXICITY TO FERTILITY

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | inhalation |
| **Exposure period** | : | 19 days |
| **Frequency of treatment** | : | 7 hours/day |
| **Duration of test** | : | 20 days |
| **Doses** | : | 150 mg/m3 |
| **Control group** | : | yes |
| **NOAEL Maternalt.** | : | = .15 mg/l |
| **NOAEL Teratogen** | : | = .15 mg/l |
| **Method** | : | other |
| **Year** | : | 1990 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ORGANISMS
Groups of approximately 15 female pregnant Sprague-Dawley rats with a mean maternal weight of 275 g at the beginning of pregnancy.

ADMINISTRATION / EXPOSURE
- Type of exposure: Inhalation, concentrations monitored continuously and recorded hourly.
- Duration of test/exposure: 7 hours a day from day 1-19 of gestation.
- Dose level: 0.4 mg/l which was the highest atmospheric concentration which could be generated at a temperature below 80F. Control animals were sham exposed.

MATING PROCEDURES: Sperm positive females used, no other information.

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily for 1st week then weekly
- Food & water consumption: Weekly on days 7, 14 and 20.
- Clinical observations: Assume daily frequency not actually reported.
- Examination of uterine content: Gestation day 20 ovaries also removed with uterus for examination of corpora lutea, implantations, resorption sites and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights and sex were recorded.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
Not carried out.

STATISTICAL METHODS: Multivariate analysis of variance (MANOVA) and ANOVA. Foetal incidence data were analysed using the Variance Test for Homogeneity of the Binomial Distribution or ANOVA. The Kruskal-Wallis test was used if a non-parametric analysis was more appropriate.

**Result** : NOAEL : 0.15 mg/l for maternal and foetal toxicity. No evidence of maternaltoxicity, foetotxicity or teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: Within 5% of the nominal concentration of 0.15 mg/l when measured by Infrared analysis. This is the highest attainable dose under the conditions of the study. Actual dose achieved 0.145 mg/l.

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Number of resorptions: Comparable in treated and control groups. Mean resorptions/litter control 0.5, treated 0.7.
- Number of corpora lutea: Comparable between treated and control groups. Mean corpora lutea/litter control 14.9, treated 13.5.
- Duration of Pregnancy: Not reported.
- Body weight: Weight gain was comparable in treated and control groups.
- Food/water consumption: Comparable between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable between treated & control groups. Mean foetuses/litter controls 13.5, treated 12.7.
- Sex ratio: No significant difference between treated and controls Controls/litter (mean) male 6.6, female 6.9; Treated/litter (mean) male 6.7, female 6.0/
- External, Soft tissue and Skeletal abnormalities: No treatment related effects. Data not presented.

**Remark** : The results reported in the primary reference (Nelson et al, 1990) are summarised in a comparative review of 13 alcohols tested by the same author (Nelson et al, 1996).

**Conclusion** : The NOAEL for maternal toxicity, foetotoxicity and teratogenicity in rats following inhalation exposure to n-nonanol during gestation (Gestation days 1-19) is 0.15 mg/l (the highest attainable concentration). There were no adverse effects on any of the maternal or foetal parameters investigated.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Nelson et al. 1990.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
06.04.2005 (7) (8) (10)

**Species** : rat
**Sex** : female
**Strain** : other: no data
**Route of admin.** : other: intragastric
**Exposure period** : gestation days 1-15
**Frequency of treatment** : daily
**Duration of test** : to gestation day 20
**Doses** : 1 ml of a 40% aqueous suspension
**Control group** : other: non standard
**Method** : other: non-standard
**Year** : 1991
**GLP** : no data
**Test substance** : other TS

**Test substance** : Nonanol was tested as part of a comparative study of C1-C10 alcohols.

**Test condition** : TEST ORGANISMS: rat initial weight 160-180g

ADMINISTRATION / EXPOSURE
- Type of exposure: intragastric
- Duration of test/exposure: gd 1-15
- Control group and treatment: 1 ml/rat water, 20 controls
- Vehicle: water
- Concentration in vehicle: 40% suspension
- Total volume applied: 1 ml/rat
- Doses: 1 ml 40% aqueous suspension (400 mg/rat) to 10 rats.

MATING PROCEDURES: Sprem positive females

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Not reported
- Food & water consumption: Not reported.
- Clinical observations: No data
- Examination of uterine content: Gestation day 20, number of corpora lutea, implantations, resorption sites, placental weight and size and live foetuses recorded.
- Examination of fetuses: Gestation day 20 examined for external, visceral and skeletal anomalies. Foetal weights were recorded.

OTHER EXAMINATIONS: Measurement of alcohol dehydrogenase in the liver of foetuses between GD 16 and postnatal day 20.

STATISTICAL METHODS: Analysis of variance.

**Result** : NOAEL : Not established, the single dose level produced evidence of foetotoxcity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL: 400 mg/rat

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None reported
- Number pregnant per dose level: Not reported
- Number aborting: Not reported
- Preimplantation loss: 12.9% (+- 3.3%) treated; 2.0% (+- 1%) controls.
- Number of resorptions: 25.0% (+- 4.6%) in treated rats); 4.4% (+- 1.4%) in controls.
- Number of corpora lutea: Comparable between treated and control groups.
- Body weight: Not reported
- Food/water consumption: Not reported
- Description, severity, time of onset and duration of clinical signs: Not reported
- Haematological findings incidence and severity: Not carried out.
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not carried out.
- Organ weight changes: Not carried out.
- Histopathology incidence and severity: Not carried out.
- Other: placental weight was not significantly affected by treatment.

FOETAL DATA:
- Litter size and weights: Not reported only total mean foetal weights reported these were significantly reduced by exposure to nonanol. Treated group foetal weight 1.76 g (+- 0.07) controls 2.25 g (+- 0.02) [p<0.001]. foetal size was also significantly reduced.
- Sex ratio: Not reported.

- External, Soft tissue and Skeletal abnormalities: No externally visible developmental anomalies. Developmental effects on the internal organs and skeleton were observed in 7.1% (+- 1.8%) of foetuses exposed to nonanol and 1.2% (+- 0.3%) of controls. These effects were not reported separately. The types of effect seen in the alcohols tested were hydrocephalus, hydronephrosis and retardation of ossification there was no indication of the frequency of these defects for each alcohol tested.
- Effect on Alcohol Dehydrogenase (ADH): Nonanol reduced the ADH level in 20 day rats by 17.2%.

**Remark** : Cited in Patty 2001 and RTECS 2004

**Reliability** : (3) invalid
Significant methodological deficiencies (small group size), analysis not conducted on a litter basis, no reporting of maternal status) coupled with insufficient documentation.

08.04.2005 (1) (10) (11)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

**Type** : other: aspiration hazard

**Remark** : Aspiration of 0.2 ml 1-nonanol produced deaths in 10/10 rats, death due to respiratory arrest was instant.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

15.09.2004 (3) (10)

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# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 85566-14-9 |
| **CAS No.** | **:** | 85566-14-9 |
| **EINECS Name** | **:** | Alcohols, C7-11-branched and linear |
| **EC No.** | **:** | 287-623-3 |

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

## 5.2.2 EYE IRRITATION

## 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

## 5.5 GENETIC TOXICITY ‘IN VITRO‘

## 5.6 GENETIC TOXICITY ‘IN VIVO‘

## 5.7 CARCINOGENITY

## 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Wistar |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | Gestation day 6-15 |
| **Frequency of treatment** | : | daily |
| **Duration of test** | : | 20 days |
| **Doses** | : | 0, 144, 720, 1440 mg/kg/day |
| **Control group** | : | yes |

| | | |
|---|---|---|
| **NOAEL Maternalt.** | : | > 1440 mg/kg bw |
| **NOAEL Teratogen** | : | > 1440 mg/kg bw |
| **Method** | : | other: OECD Guidelines 414 and EEC directives 87/302/EEC and 67/548/EEC |
| **Year** | : | 1997 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | C7-9-11 alcohol CAS RN 85566-14-9 >= 99% pure 65% linear |
| **Test condition** | : | TEST ORGANISMS<br>- Groups of 8-10 pregnant Wistar rats aged 68-85 days at study initiation, mean weight 214-233 g<br><br>ADMINISTRATION / EXPOSURE<br>- Type of exposure: gavage<br>- Duration of test/exposure: treatment day 6-15 post coital, termination day 20 post coital.<br>- Treatment: 0, 144, 720 or 1440 mg/kg/day<br>- Control group and treatment: two control groups were used one with twice distilled water and one with 0.005% Cremophor EL as emulsifier.<br>- Vehicle: 0.005% Cremophor in water<br>- Concentration in vehicle: Adjusted to give constant volume<br>- Total volume applied: 5 ml/kg<br><br>MATING PROCEDURES: 1 fertile male to 4 females.<br><br>PARAMETERS ASSESSED DURING STUDY:<br>- Body weight gain: Daily<br>- Food consumption: Daily<br>- Clinical observations: Daily<br>- Examination of uterine content: At gestation day 20, uterine weight, numbers of implantations shown as: live foetuses, dead implantations, early resorptions (stained), early & late resorptions (unnstained), dead foetuses. Conception rates and pre & post implantational losses were calculated.<br>- Examination of fetuses: Foetal weights, external, visceral and skeletal anomalies, variations & retardations, unclassified observations.<br><br>ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):<br>Not reported<br><br>STATISTICAL METHODS: Dunnetts test for most reproductive parameters and Fischers exact test for evaluaton of conception rate and all foetal findings. |
| **Result** | : | NOAEL: The NOAEL for maternal toxicity, teratogencity and foetotoxicity is 1440 mg/kg/day . There were no treatment related effects on the dams or foetuses.<br><br>ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 144, 720 and 1440 mg/kg/day<br><br>MATERNAL TOXIC EFFECTS BY DOSE LEVEL:<br>- Mortality and day of death: None<br>- Number pregnant per dose level: water control 9, aqueous emulsifier 10, 144 mg/kg 9, 1440 mg/kg 8.<br>- Number aborting: None<br>- Number of resorptions: Comparable in treated and control groups. |

Resorptions/dam (mean) 1.2, 1.1 (control groups) 1.0, 1.2 and 1.1 for low, mid and high dose groups.
- Number of implantations: Comparable in treated and control groups. Implantation sites/dam (mean) 15.0, 15.7 (control groups) 14.8, 15.8 and 13.9 for low, mid and high dose groups.- Post implantation loss: Comparable in treated and control groups.
- Number of corpora lutea: Comparable in treated and control groups. Corpora lutea/dam (mean) 16.1, 16.0 9control groups) 17.0, 17.0 and 15,6 for low, mid and high dose groups.
- Duration of Pregnancy: Comparable in treated and control groups.
- Body weight: Comparable in treated and control groups.
- Food/water consumption: Comparable in treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None
- Hematological findings incidence and severity: not carried out
- Clinical biochemistry findings incidence and severity: Not carried out.
- Gross pathology incidence and severity: Not reported
- Organ weight changes: Uterine weight and placental weight was unaffected by treatment.
- Histopathology incidence and severity: Not carried out.

FETAL DATA:
- Litter size and weights: Comparable in treated and control groups. Foetal weights (mean) 3.8, 3.82 (controls) 3.88, 3.79 and 3.82 for low, mid and high dose groups.
- Number viable: Viability was comparable to controls. Live foetuses/dam (mean) 13.8, 14.6 (controls) 13.8, 14.6 and 12.8 - Sex ratio: Not reported.
- Total malformations, variations and retardations: The incidence was unaffected by treatment. Incidence comparable between treated and control groups. Litters (%) with malformations (no of litters) 11.1 (1), 20.0 (2)(controls) 11.1 (1), 40.0 (4) and 12.5% (1) for low, mid and high dose groups. Litters (%) with variations (no of litters) 88.9 (8), 100 (10) (controls) 100 (9), 100 (10) and 100% (8) for low, mid and high dose groups. Litters (%) with retardations (number of litters) 88.0 (8), 100 (10) (controls) 77.8 (7), 90.0 (9) and 87.5% (7)

**Conclusion** : There were no adverse effects on maternal toxicity, reproductive parameters or foetal endoints at any of the dose levels tested following administration to rats by gavage on gestation days 6-15 (C7-9-11 alcohol). The NOAEL for maternal toxicity, teratogenicity and foetotoxicity is >1440 mg/kg/day (highest dose level tested).

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Hellwig & Jackh, 1997

**Flag** : Critical study for SIDS endpoint

10.08.2005 (1)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

(1) Hellwig, J. and Jackh, R. 1997. Differential prenatal toxicity of one straight-chain and five branched-chain primary alcohols in rats. Food and Chem. Toxicol. 35:489-500

# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

Note: References in this file are given separately for physicochemical properties, environmental fate, ecotoxicology (i.e. chapters 2-4) and human health endpoints (chapter 5).

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 112-53-8 |
| **CAS No.** | **:** | 112-53-8 |
| **EINECS Name** | **:** | dodecan-1-ol |
| **EC No.** | **:** | 203-982-0 |
| **TSCA Name** | **:** | 1-Dodecanol |
| **Molecular Formula** | **:** | C12H26O |

## 2.1 Melting Point

**Value:** = 22.6 - 24 degree C

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Budavari 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (2)

## 2.2 Boiling Point

**Value:** = 255 - 269 degree C

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (25)

**Value:** = 259 degree C at 1013 hPa

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Budavari 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (2)

## 2.3 Density

**Value:** = .83

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** SIDS Dossier on 1-Dodecanol 1993a.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (19)

**Value:** = .83 at 20 degree C

## 2.4 Vapour Pressure

**Value:** = .00113 hPa at 25 degree C

**Method:** other (measured)
**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Daubert and Danner 1989.
**Reliability:** (2) valid with restrictions
30-SEP-2003 (4)

**Value:** = .0087 hPa at 20 degree C

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Verschueren 1996.

**Reliability:** (4) not assignable
30-SEP-2003 (25)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 5.36

**Method:** other (measured)
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
**Source:** Burkhard et al. 1985.
**Test condition:** ambient temperature
**Reliability:** (2) valid with restrictions
01-OCT-2003 (3)

**Partition Coeff.:** octanol-water
**log Pow:** = 5.13

**Test substance:** other TS: Dodecanol (112-53-8)

Method other (measured)
**Source:** SRC.
**Reliability:** (4) not assignable
01-OCT-2003 (20)

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = 1.7 - 2.9 mg/l

**Method:** other
**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** Solubility in water = 1.7 mg/l @ 16 C to 2.9 mg/l @ 34 C
**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
29-OCT-2003 (25)

**Solubility in:** Water
**Value:** = 1.93 mg/l at 20 degree C

**Method:** other: measured (slow stir procedure)
**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Letinski 2002.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (13)

**Solubility in:** Water
**Value:** = 4 mg/l at 25 degree C

**Method:** other (measured)
**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** SRC.
**Reliability:** (4) not assignable
29-OCT-2003 (20)

**Solubility in:** Water
**Value:** = 1.9 mg/l at 25 degree C

**Method:** other: measured (GC)
**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Veith et al.1983a.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (23)

## 2.9 Flammability

**Result:** flammable

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** SIDS Dossier on 1-Dodecanol 1993a.
**Reliability:** (2) valid with restrictions
19-AUG-2003 (19)

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent of predominantly domestic sewage treatment plant
**Concentration:** 2 mg/l related to Test substance
**Contact time:** 28 day(s)
**Degradation:** = 79 % after 28 day(s)
**Result:** readily biodegradable

**Method:** OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** EEC-Directive 92/69/EEC Annex V, Part C: Methods for the Determination of ecotoxicity. C.4. Biodegradation: determination of the 'ready biodegradability' C.4-E
This method corresponds to OECD test method 301D.
**Remark:** The following validity criteria were fulfilled (1) the reference substance reached the pass level of 60% within 14 days. (2) Parallel assays did not differ by greater than 20%. (3) Residual concentration of O2 in test bottles did not fall below 0.5 mg/l. (4) O2 depletion in the blanks was less than 1.5 mg/l after 29 days.
**Result:** 7 days = 54%
14 days = 68%
21 days = 80%
28 days = 79%
The test substance (2 mg/l) attained >60% degradation during the 14 day window. The values reported in the results section are for the 2 mg/l concentration. The 5 mg/l concentration of test substance had insufficient residual dissolved oxygen content after 21 days.
**Source:** Richterich 1993.
**Test condition:** INOCULUM/TEST ORGANISM
Sampling site: Plant Hochdahl, Germany
INITIAL TEST SUBSTANCE CONCENTRATION: 2 and 5 mg/l
METHOD OF PREPARATION OF TEST SOLUTION: an inert emulsifier (nonylphenol ethoxylated propoxylated, NP+9.5 EO+5PO) was used to disperse the test substance. Concentration of emulsifier not reported.
ANALYTICAL PARAMETER: Chemical Oxygen Demand (COD)
TEST CONDITIONS:
- Composition of medium: not reported
- Additional substrate: none
- Test temperature: 20 +/- 1C
- pH value: not reported
- Aeration of dilution water: not reported
- Concentration of suspended solids: not reported
INTERMEDIATES/DEGRADATION PRODUCTS: not reported
NITRATE/NITRITE MEASUREMENT: yes
CONTROLS: mineral medium/ mineral medium with inoculum/ mineral medium with inoculum and emulsifier. Degradation

rate of test substance was corrected by oxygen uptake of blank inoculum and emulsifier control.
REFERENCE SUBSTANCE: Sodium benzoate

**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
03-NOV-2003 (17)

**Type:** aerobic
**Inoculum:** activated sludge
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Degradation:** = 100 % after 28 day(s)
**Result:** readily biodegradable

**Method:** other: ISO 10708 (BODIS)
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken.
**Remark:** Total oxygen uptake in flasks is calculated from blank-corrected decrease in measured dissolved oxygen concentration divided by saturation value at normal conditions and multiplied with total oxygen content originally present in liquid and gas phase.
The following validity criteria are met (1) Parallel assays did not differ by more than 20%, (2) reference compound reached the pass level within 14 days and (3) residual concentration of oxygen did not fall below 0.5 mg/l. It could not be determined whether oxygen depletion in the blank exceeded 1.5 mg/l after 28 days as no data for day 0 was included.
**Result:** 7 days = 72%
14 days = 89%
21 days = 93%
28 days = 100%
The substance degraded >60% in the 10 day window. The reference substance, Sodium acetate trihydrate, degraded 86% over the 28 day period.
**Source:** Henkel KGaA 1992c.
**Test condition:** Concentration of activated sludge: 30 mg dry matter/l
Test volume: 200 ml
Temperature: 20-25 C
pH: not reported
**Test substance:** This test substance corresponds to CAS # 112-53-8. Tradename is Lorol C12-99.
**Reliability:** (1) valid without restriction
Not key study: Other study with same reliability score and using OECD 301D methodology exists.

29-OCT-2003 (8)

**Type:** aerobic
**Inoculum:** activated sludge, domestic, non-adapted
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 46 day(s)
**Degradation:** = 71 % after 28 day(s)
**Result:** readily biodegradable

**Method:** other: Sturm 1973
**Year:** 1991
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** This test method corresponds to OECD 301B
**Remark:** The following validity criteria were met: (1) the blanks were valid for this test, the maximum milligrams of carbon dioxide were well within the 40 mg/l range, (2) both sodium acetate samples obeyed the 10-60% rule, no days were required for the bacterial population to acclimate to the sodium acetate, (3) Parallel assays did not differ by more than 20%.
**Result:** 4 days = 16%
8 days = 44%
14 days = 60%
28 days = 71%
46 days = 73%
Report states that both ALFOL 12 alcohol samples obeyed the '10-day window' rule and 3 days were required for the bacterial population to acclimate to the alcohol. The reference substance, Sodium acetate, degraded by 78% after 28 days.
**Source:** Morris et al. 1991.
**Test substance:** The test substance corresponds to CAS# 112-53-8. Tradename is Alfol 12.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and a with higher degradation rate are available.
25-SEP-2003 (16)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 26 mg/l related to Test substance
**Degradation:** = 50 % after 28 day(s)
**Result:** inherently biodegradable

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1996
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** Test solutions were prepared and inoculated in 5 l glass vessels each containing 3 litres of solution. Each test vessel was inoculated with the prepared inoculum at a final concentration of 30 mg suspended solids (ss)/l. The study was carried out at a temperature of 21 C in darkness.
**Remark:** The following validity criteria were met (1) the IC content of the test substance suspension in the mineral medium at the beginning of the test was less than 5% of the total carbon, (2) parallel assays did not differ by more than 20%, (3) reference compound reached the pass level within 14 days, (4) Total Co2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test.
**Result:** 6 days = 8%
14 days = 27%
20 days = 48%
28 days = 50%

The test substance degraded <60% during the 10 day window. The reference substance, Sodium benzoate degraded by 105% after 28 days.
**Source:** Mead 1997a.
**Test substance:** This substance corresponds to CAS# 112-53-8. Tradename is Kalcol 2098.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
10-SEP-2003 (15)

**Type:** aerobic
**Inoculum:** other: no information provided on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 41 % after 31 day(s)
**Result:** inherently biodegradable

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** There is no information given on the validity criteria.
**Result:** 4 days = 11%
10 days = 26%
17 days = 34%
24 days = 38%
31 days = 41%
The test substance attained <60% degradation during the 10 day window. Sodium benzoate was used as a positive control and reached a mineralization extent of 62.2%.
**Source:** Vista 1994.
**Test substance:** The substance corresponds to CAS# 112-53-8. Tradename is ALFOL 12.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but with higher degradation rates are available.
18-SEP-2003 (27)

## 3.6 BOD5, COD or BOD5/COD Ratio

**Method:** other: APHA 1980
**GLP:** no data
**Year:**
**Method:** Test chemical and 1 ml of acclimated seed were added to 20 ml of dilution water in 300 ml BOD bottles. The bottles were then filled to capacity with dilution water, sealed, and incubated for 5d at 21 C +/- 3 C. Initial concentrations of

test chemical in the BOD bottles ranged from 0 to 3.2 mg/l and never exceeded the measured (or in some cases, estimated) water solubility of the chemical.

**Remark:** The primary purpose of this study was to determine a quantitative structure-biodegradability relationship for a series of alcohols.

**Result:** 23.2% degradation after 5 days (% ThOD)

**Source:** Vaishnav et al. 1987.

**Test substance:** Dodecanol (112-53-8)

**Reliability:** (2) valid with restrictions

13-AUG-2003 (22)

## 3.7 Bioaccumulation

**BCF:** = 3801

**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** The modeled result reported in the 1993 Dossier is considerably higher than the modeled result using the EPISuite model in 2000.

**Source:** SIDS Dossier 1993a.

**Reliability:** (2) valid with restrictions

25-SEP-2003 (19)

# AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

**Type:** flow through
**Species:** Pimephales promelas (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** yes
**LC50:** = 1.01
**Limit Test:** no

**Method:** other: USEPA 1975
**Year:** 1983
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Result:**
RESULTS: EXPOSED
LC50 = 1.01 mg/l
Based on measured results
RESULTS: CONTROL
Number/% showing adverse effects: Not reported
The publication indicates all concentrations were monitored daily using analytical methods, however, no results are included.

**Source:** Veith et al. 1983a; Veith et al. 1983b.

**Test condition:**
TEST ORGANISMS
Strain: Pimephales promelas
Supplier: Environmental Research Laboratory-Duluth culture
Weight: 0.12 g
Age: 30 days old
Feeding: not reported
Pretreatment: not reported
Feeding during test: none
Control group: 2 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none
Concentration of vehicle, solvent: none
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: Lake Superior
Aeration: not reported
Alkalinity: 42.2 mg/L
Hardness: 56.3 mg/L CaCO3
Conductance: Not reported
TEST SYSTEM
Concentrations: 5 different concentrations
Renewal of test solution: not reported
Exposure vessel type: Test tanks
Number of replicates: 2
Fish per replicate: 2
Test temperature: 25 C
Dissolved oxygen: > 60% of saturation
pH mean: 7.5
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: not reported

TEST PARAMETER: Mortality
SAMPLING: Deaths recorded at 1, 3, 6, 12, 24, 48, 72 and 96h.
MONITORING OF TEST SUBSTANCE CONCENTRATION: Concentrations of chemicals in water were measured in each tank throughout the test.

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
12-MAR-2004 (23) (24)

**Type:** semistatic
**Species:** Oncorhynchus mykiss (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** >= 1
**LC50:** > 1
**Limit Test:** yes

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1996
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** 2 groups of 10 fish were exposed to an aqueous dispersion of the test material at a single concentration of 1.0 mg/l. Mortalities and sub-lethal effects of exposure were determined at 3 and 6 hours after the start of the test and then daily until termination at 96 hours.
**Source:** Wetton 1996a.
**Test substance:** Corresponds to tradename Kalcol 2098.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
12-MAR-2004 (28)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = .316
**EC50:** = .765
**EC100:** = 1.78
**Limit Test:** no

**Method:** OECD Guide-line 202
**Year:** 1997
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** The test substance was water-insoluble, however, a fine-turbid suspension could be prepared using slightly prewarmed demineralised water (23 C to 25 C). The test substance and prewarmed water were placed into vessels and were shaken manually for 3 minutes. The resulting suspension remained stable even at temperatures of 20 C and could be diluted. The suspensions were not filtered. Note, effects seen at concentration less than SPARC estimated water

solubility.
The tests reported in this entry used a standard methodology. An additional test was also carried out using a non-standard submergible chamber procedure. Test concentrations were 0.316, 0.562, 1.00, 1.78, 3.16 and 5.62 mg/l. The EC50 was determined to be 1.589 mg/l based on nominal concentrations.

**Result:** RESULTS: EXPOSED
EC0 = 0.316 mg/l
EC50 = 0.765 mg/l
EC100 = 1.78 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Laboratory of Pharmacology and Toxicology 1997.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Institut fur Wasser-, Boden-, und Lufthygiene
Age: 6-24 hours old
Feeding: Algae and a small amount of aerated sewage
Pretreatment: None
Feeding during test: None
Control group: 1 control group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: None
Concentration of vehicle, solvent: None
STABILITY OF TEST CHEMICAL SOLUTIONS
No analysis
DILUTION WATER
Source: Reconstituted, aerated, fully demineralised water
Aeration: Not reported
Alkalinity: 0.8 mmol/l
Hardness: 250 mg CaCO3/l
Conductance: Not reported
TEST SYSTEM
Concentrations: 0.178, 0.316, 0.562, 1.00, 1.78, and 3.16 mg/l
Renewal of test solution: None
Exposure vessel type: all glass vessels , diameter: 38 mm, height: 60 mm, volume: 50 ml
Number of replicates: 4
Invertebrate per replicate: 5
Test temperature: 20 C
Dissolved oxygen: >80% of maximum saturation
pH mean: 7.9
Adjustment of pH: None
Intensity of irradiation: Not reported
Photoperiod: 16 hours light/8 hours darkness
white type fluorescent light
TEST PARAMETER: Immobilization
MONITORING OF TEST SUBSTANCE CONCENTRATION: None

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

12-MAR-2004 (12)

**Species:** Daphnia magna (Crustacea)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = .45

**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** Indicated in table as unpublished results (S Marshall, Unilever Research). Test solutions were prepared using sonication but no solvents.
**Source:** Unilever, 1995.
**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available, data obtained from secondary literature
12-MAR-2004 (21)

**Type:** static
**Species:** Nitocra spinipes (Crustacea)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC50:** = 1
**Limit Test:** no

**Method:** other
**Year:** 1984
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** The acute mortality tests were carried out under static conditions. Tests were carried out in at least six concentrations and one control. Twenty invertebrates were exposed to each concentration. Water was maintained at pH 7.9 and 10 C.
**Remark:** This entry was originally reported in Linden et al 1979. However, the later study (Bengtsson et al 1984) is specific to the aliphatic alcohols which were tested and provides more detail.
**Source:** Bengtsson, 1984
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity but with standard test organisms are available
12-MAR-2004 (1) (14)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC0:** = 100
**EC50:** = 320
**EC100:** = 1000
**Limit Test:** no

**Method:** other
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11).
This method corresponds to the OECD Guideline 202, part 1.
**Source:** Henkel KGaA 1999q

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
12-MAR-2004 (11)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: biomass and growth rate
**Exposure period:** 72 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EbC0 :** = .4
**EbC50 :** = .62
**ErC50 :** = 2.6
**Limit Test:** no

**Method:** other: DIN 38412, Part 9 (Conforms with OECD-Guideline 201.).
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Henkel KGaA 1994d.
**Test condition:** TEST ORGANISMS
Strain: Scenedesmus subspicatus SAG 8681
Supplier: Institute of Plant Physiology, University of Gottingen
Pretreatment: not reported
Controls: 3 flasks served as controls
Initial cell concentration: 1*10exp4 cells/ml
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Ethanol
Concentration of vehicle, solvent:
STABILITY OF TEST CHEMICAL SOLUTIONS:
REFERENCE SUBSTANCE:
TEST SYSTEM:
Test type: static test
Loading rates: 0.1, 0.2, 0.4, 0.8, 1, 2, 4 and 8 mg/l
Renewal of test solution: None
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Test temperature: 21.9-22.6 C
pH mean: 7.5-8.1
Intensity of irradiation: 2000lux
Photoperiod: continuous illumination
TEST PARAMETER: biomass and growth rate
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
13-JAN-2004 (10)

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** other: growth rate and biomass
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** = .3
**EbC0 :** = .3
**EbC10 :** = .73
**EbC50 :** = .97
**Limit Test:** no

**Method:** other: DIN 38412, Part 9 (Conforms with OECD-Guideline 201.).
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** Reported data refers to the effects on biomass only. The data referring to the effect on growth rate, show that up to the highest test substance concentration (10 mg/l) only <=30% inhibition was observed. Therefore, no ErC50 value was calculated in this study.
**Result:** RESULTS: EXPOSED
Biomass
EbC10 (0-72h) = 0.79 mg/l
EbC10 (0-96h) = 0.73 mg/l
EbC50 (0-72h) = 6.02 mg/l
EbC50 (0-96h) = 0.97 mg/l
**Source:** Henkel KGaA 1992.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but showing greater toxicity are available
13-JAN-2004 (7)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** = 6.25

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultured S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
**Source:** Hattori 1987.
**Reliability:** (3) invalid
Study was considered invalid due to significant methodological deficiencies.
30-OCT-2003 (6)

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** > 10000

**Method:** other
**Year:** 1994
**GLP:** yes

**Test substance:** other TS: Dodecanol (112-53-8)

**Remark:** German standard methods for the examination of water, waster water and sludge; bioassays (group L); determination of the inhibitory effect of waste water on the oxygen consumption of Pseudomonas putida (L 27); DIN 38412 part 27.
The oxygen consumption rate of a bacterial suspension fed glucose as nutrient base is measured after a contact time of 30 minutes. The oxygen consumption rate of the same bacterial suspension in the presence of various concentrations of a test substance under otherwise identical conditions is also measured.
This information is additional to that reported in the 1993 SIDS dossier for dodecanol prepared by the Danish Ministry of the Environment.
**Source:** Henkel KGaA, 1994b
**Test substance:** This substance corresponds to CAS # 112-53-8. Tradename is Lorol 12-99.
**Reliability:** (1) valid without restriction
Best study although not a SIDS endpoint.
30-OCT-2003 (9)

**Species:** Tetrahymena pyriformis (Protozoa)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:**
**NOEC:** = 1.15
**EC50:** = 1.58
**EC100 :** = 2

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
01-OCT-2003 (25)

**Species:** other bacteria: Mycoplasma gallisepticum
**Exposure period:** 6 day(s)
**Unit:** mg/l **Analytical monitoring:**
**NOEC:** = 11.9

**Test substance:** other TS: Dodecanol (112-53-8)

**Source:** Verschueren 1996.
**Reliability:** (4) not assignable
Not key study: Other studies with higher reliability score are available
01-OCT-2003 (25)

## 4.5 Chronic Toxicity to Aquatic Organisms

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** Survival, growth and reproduction rate
**Exposure period:** 21 day(s)

**Unit:** ug/l
**Analytical monitoring:** yes
**NOEC:** 14
**LOEC:** 95
**EC10:** 13
**EC20:** 34

**Method:** OECD 211
**Year:** 2005
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:**

GUIDELINE: OECD 211 with modifications to allow aeration of exposure media.

STATISTICS: The evaluation of the concentration-effect-relationships and the calculations of effect concentrations were based on mean measured initial concentrations as multiple peak concentrations, as well as on geometric means between mean measured initial and aged (24h) test concentrations. For each endpoint, the NOEC, LOEC, and, if possible, the EC50, EC20 and EC10 were determined. A LOEC and NOEC were calculated by ANOVA followed by Williams' test or an appropriate non-parametric test suggested by the ToxRat program. When the test results showed a concentration-response relationship, the data were analysed by regression using Probit-analysis assuming log-normal distribution of the values using the computer program ToxRat program.

TEST CONCENTRATIONS: Nominal test concentrations were 0, 25, 69, 185 and 500 µg test item/L. Mean measured concentrations of freshly prepared test solutions were <Limit of quantification, 20, 56, 163 and 534 µg/L. The geometric means of mean measured initial and aged concentrations after 24 h hours were <Limit of quantification, 3, 5, 14 and 95 µg/L.

TEST MEDIUM PREPARATION: Test solutions were prepared daily by stirring the test substance in test media under slow stir conditions (21 h) in sterilized mixing vessels. The mixing vessels were cylindrical brown glass bottles with teflon covered screw caps, fitted with a drain port near the bottom for drawing off the test solution. The volume of the mixing vessels was 2 L. After stirring, the contents of the vessels were left to settle for 2 h. The saturated aqueous phase was then taken out of the drain port. The first fraction 0-100 mL was discarded. The fraction between 100 and 1800 mL was used for rinsing (200 mL) and filling (1000 mL) the test flasks for toxicity testing and for analytical measurements (500 mL), if done. Rinsing of the test vessels was carried out to saturate the surfaces of the test vessels. After filling, the vessels were closed immediately by using autoclaved silicone stoppers and only opened to introduce the test organisms and again at the renewals of the test media. The test media were not stored for more than 1 - 2 hours prior to testing

EXPOSURE REGIME: Semi-static, daily renewal. As a deviation from OECD Guideline 211, all test vessels were aerated with sterile filtrated synthetic air: the autoclaved silicone stoppers were fitted with fine glass capillaries connected to the aeration unit. The aeration was necessary to avoid severe

oxygen depletion due to the increase of transferred bacteria with growing Daphnia magna as observed in pre-studies and the associated oxygen consumption by the degradation of the test substance.

TEST ORGANISMS: *Daphnia magna* STRAUS, Crustacea, Cladocera. Age: 4 - 24 hours old. Origin: Umweltbundesamt (German Federal Environment Agency). Test organisms bred in the laboratory of the Fh-IME (testing facility).

TEST APPARATUS: Each *Daphnia magna* was exposed separately in a numbered vessel flask) containing 100 mL of test medium.

FEEDING: The *Daphnia magna* were fed at each renewal with suspensions of unicellular green algae. The suspensions of *Desmodesmus subspicatus* (daily prepared from axenic cultures) were controlled analyzed for microbial contamination one and two weeks after test start by using "Cult-Dip combi® Dip Slides (Merck)". No bacterial contamination was detected. The content of food in the test suspensions, measured as turbidity at 758 nm, increased during the test from 7 mg C/L equivalents to
15 mg C/L equivalents.

TEST DESIGN: For each test concentration and for the control 10x1 animals were used.

TEST CONDITIONS: The vessels were subjected to a light/dark cycle of 16/8 hours. The test temperature during the test was in the range 21.0 to 22.0°C, the light intensity was in the range 585 to 647 lux. The oxygen saturation never fell below 56 % (4.0 mg/L), and the mean pH was 9.3 to 9.5 at all treatment levels.

ENDPOINT OBSERVATIONS: The parent *Daphnia magna* were assessed visually daily for immobility and any other abnormalities in appearance and behaviour. At study termination, the length of the adults was measured by digital photography and image analysis and their statistics compared with those of the control animals. The newborn *Daphnia magna* in each beaker were counted at each daily renewal of the test solutions, inspected for abnormalities in condition, and removed. The following endpoints observed in the reproduction test were evaluated quantitatively:
• Mortality (immobility) of parental generation *Daphnia magna*
• Age at first brood
• Total number of offspring per replicate
• Cumulative Number of live offspring per surviving female at the time of recording
• Intrinsic rate of increase, r
• Individual length of adults

ANALYSIS OF TEST MEDIA: All the test concentrations were sampled for chemical analysis three times a week at renewal of the test media. A 500 mL aliquot of the fresh solutions was used for analysis. After 24 h, at the next renewal, the aged test liquids were pooled (vessels 1- 5 and 6-10) and analysed. The analyte was extracted from the aqueous test samples by liquid-liquid partitioning with n-hexane. After derivatization of the analyte by MSTFA measurement was performed by GC-MS using n-dodecanol-d25 as internal standard. The method was

validated for the determination of the test item in *Daphnia* test medium in the concentration range of 1.0 - 100 µg/L

**Result**: SURVIVAL, GROWTH AND REPRODUCTION DATA

| Test item nominal conc. (µg/L) | Survival (%) | Growth (length) Mean ± SD (mm) | Age at first brood Mean ± SD (days) |
|---|---|---|---|
| Control | 100 | 4.83 ± 0.35 | 8.2 ± 0.79 |
| 25 | 100 | 4.37 ± 0.39 | 8.2 ± 0.92 |
| 69 | 100 | 4.47 ± 0.31 | 8.4 ± 0.84 |
| 185 | 100 | 4.38 ± 0.41 | 8.1 ± 0.99 |
| 500 | 40 | 4.76 ± 0.40 | 8.6 ± 1.14 |

| Test item nominal conc. (µg/L) | Cumulative offspring per female Mean ± SD (#) | Intrinsic rate of increase r Mean ± SD (1/d)) |
|---|---|---|
| Control | 68.0 ± 8.9 | 0.320 ± 0.024 |
| 25 | 68.0 ± 11.6 | 0.319 ± 0.026 |
| 69 | 63.0 ± 9.8 | 0.307 ± 0.018 |
| 185 | 61.0 ± 7.1 | 0.304 ± 0.019 |
| 500 | 64.0 ± 19.3 | 0.256 ± 0.044 |

CALCULATED STATISTICS:

Related to daily initial concentrations:
EC10 = 150 µg test item/L
EC20 = 520 µg test item/L
LOEC = 530 µg test item/L
NOEC = 160 µg test item/L

Related to mean measured concentrations:
EC10 = 13 µg test item/L
EC20 = 34 µg test item/L
LOEC = 95 µg test item/L
NOEC = 14 µg test item/L

**Test substance:** C12 Fatty alcohol (1-Dodecanol)
CAS No. 112-53-8
Sample received from Laboratory Dr. Ehrenstorfer-Schafers, Augsburg, Germany.
Lot No: 30403
Purity: 98.0 % ± 0.5 %

**Reliability:** (1) Reliable without restrictions
Guideline study conducted in accordance with GLP.
**Flag** Critical Study for SIDS endpoint

(18)

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: reproduction rate and mortality
**Exposure period:** 21 day(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** = 1
**LOEC:** = 3

**Method:** other: Comparable to OECD guideline 202, Part 2.
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** Chronic toxicity testing in Daphnia magna according to UBA toxicity testing protocol 'Prolonged toxicity test with Daphnia Magna', 01.02.1984; determination of the NOEC for reproduction rate, mortality and the moment of the first appearance of descendants.
**Remark:** Data refers to both mortality of parents and number of offspring/parent. The test substance was added directly, without the use of solvents. The aqueous solubility of Dodecanol is 3 mg/l. Effects of mortality were all seen in dose groups above the limit of saturation.
**Result:** RESULTS:

| Concentration (mg/L) | 0 | 1 | 3 | 10 | 30 | 100 |
|---|---|---|---|---|---|---|
| First day of offspring | 9-12 | 9-12 | 9-12 | 9-12 | 9-12 | 9-12 |
| Survival rate of adults (%) | 90 | 90 | 90 | 50 | 45 | 40 |
| Average number of young animal per adult | 106 | 112 | 84 | 55 | 25 | 28 |
| Standard deviation | 3.6 | 3.5 | 13.2 | 15.3 | 12.6 | 4.3 |
| Significant (p<0.05) | -- | no | yes | yes | yes | yes |

NOEC = 1 mg/L
LOEC = 3 mg/L

CONTROL SUBSTANCE:
No use of control substance reported.
**Source:** Guhl 1992.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Own breeding, strain is identical with that of BGA
Age: not reported
Feeding: 1 ml algae (1-3* 10E6 cells/ml) and 1 ml activated sludge
Feeding during test: Monday/Wednesday/Friday
Control group: 1 group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none (test substance was weighed directly into test vessels)
Concentration of vehicle/solvent: not applicable
DILUTION WATER
Source: aerated tap water
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 1, 3, 10, 30 and 100 mg/l
Renewal of test solution: Test solutions changed 3 times per week (Mondays/Wednesdays/Fridays)
Exposure vessel type: 500 ml Erlenmeyer Flasks
Number of replicates: 4
Animals per replicate: 5
Test temperature: 21.5 - 22 C
Dissolved oxygen: 90-92% saturation

pH mean: 8.3-8.5
Intensity of irradiation: Radium 60W
Photoperiod: 16 hours light, 8 hours dark
TEST PARAMETER: reproduction rate and mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: Measured DOC concentrations at 0, 48 and 120 hours. The mean measured (DOC) concentrations in the 10 mg/l group were 0.55, 1.25 and 1.85 mg/l at 0, 48 and 120 hours respectively. Similar measured concentrations were observed in the 30 and 100 mg/l groups.

**Reliability:** (2) valid with restrictions
30-OCT-2003 (5)

**Species:** other: Brachionus calyciflorus (rotifer)
**Endpoint:** mortality
**Exposure period:** 2 day(s)
**Unit:** mg/l **Analytical monitoring:** yes
**EC50:** = .81 - .88

**Method:** other
**Year:** 1996
**GLP:** no data
**Test substance:** other TS: Dodecanol (112-53-8)

**Method:** Test based on modified method of Snell and Moffat (A 2-d life cycle test with the rotifer Brachionus calyciflorus, Environ. Toxicol. Chem. 11:1249-1257 (1992)).
Modifications of the diet, water source and light level were made to better reflect conditions in the natural environment.
**Remark:** In repeat tests the EC50 values for Dodecanol were 0.81 and 0.88 mg/l.
The 2-day rotifer test is considered a chronic test because multiple broods are produced and the F1 generation produces neonates
**Result:** RESULTS: EXPOSED
Test 1
EC20 = 0.74 mg/l
EC50 = 0.81 mg/l
Test 2
EC20 = 0.71 mg/l
EC50 = 0.88 mg/l
Based on measured concentrations
RESULTS: CONTROL
Number/percentage of animals showing adverse effects:
Not reported
**Source:** Versteeg 1997.
**Test condition:** TEST ORGANISMS
Strain: Brachionus calyciflorus
Supplier: Bioresponse Systems Inc., Halifax, NS, Canada
Age: <3 hours old
Feeding: Algae, Selenastrum capricornutum and Chlorella vulgaris cultured in Bold's basal media were used to feed Rotifers
Pretreatment: Approximately 3000 cysts were hydrated with dilution water 20h prior to test initiation
Feeding during test: Newly hatched swimming rotifers were placed in 10 ml of test water containing an equal mixture of C. vulgaris and S. capricornutum at 1 * 10 6 cells/ml

Control group: 1 control group and solvent group, if appropriate (3 replicates in each)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle/solvent: not reported
DILUTION WATER
Source: 50/50 blend of locally obtained well water and deionised water
Aeration: not reported
Alkalinity: not reported
Hardness: 152 mg/l CaCO3
Conductance: 450 umhos
TEST SYSTEM
Concentrations: 4-6 test concentrations up to the limit of solubility
Renewal of test solution: none
Exposure vessel type: not reported
Number of replicates: 3
Animals per replicate: 6
Test temperature: 25 +/- 2 C
Dissolved oxygen: 8.5 mg/l
pH mean: 8.6
Adjustment of pH: not reported
Photoperiod: 16/8 h light:dark cycle under low light conditions
TEST PARAMETER: mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: measured daily, overall test concentrations decreased by 20 to 90% over the 2 day test period, however concentrations for individual compounds not reported.

**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.

25-SEP-2003 (26)

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**Test substance** : n-octyl alcohol; n-decyl alcohol, lauryl alcohol and cetyl alcohol all radiolabelled (1-C14) and >98% pure.

**Test condition** : Groups of 3 hairless mice were used. The 1-C14 labelled test substances were applied to the dorsal skin using a plaster for a 24 hour period. Immediately following application of the test material each animal was placed in a container to measure expiratory excretion. At the end of the exposure period the treated area of skin was excised and dissolved using tissue solubiliser. The carcass was homogenised in a blender wwith sodium hydroxide. An aliquot of the homogenate was then dried and combusted for determination of radioactivity.

The effect of different solvents and concentration of the solvent was also investigated. The role of skin irritation in absorption of test substance was also examined.

**Result** : Distribution results were reported for lauryl alcohol (98% pure). 95% of the dose adminstered was recovered from the application site at 24 hours after dosing. 0.13% remained in the body while 0.10% was excreted in the urine and faeces. 2.61% was excreted in expired air as CO2. The ratio of the amount of compound excreted via expired air to the amount absorbed is the expiratory excretion rat. It was 91% for lauryl alcohol. The respiratory excretion rates for all the other alcohols investigated were >65% although all the actual data is not reported.

Absorption decreased with increasing carbon chain length. The absorption rate was investigated in different solvents (squalene, castor oil, triethyl citrate (TEC). The percutaneous absorption rate of undiluted n-octanol was 50%, this was increased in squalene but decreased in castor oil or TEC. This was also reported with the other alcohols tested and the tendency was more pronounced at higher concentrations.

The degree of skin irritation was proportionally related to the degree of percutaneous absorption.

**Conclusion** : Following skin application of lauryl alcohol about 2.84 % of the administered dose was absorbed. Of this absorbed dose >90% was excreted in expired air (CO2). A similar trend was observed with the other alcohols tested. Absorption decreased with increasing carbon chain length and was affected by solvent and concentration.

**Reliability** : (2) valid with restrictions

**Source** : Iwata et al, 1987
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

25.11.2004 (16)

**Test substance** : As prescribed Lauryl alcohol

**Remark** : Lauryl alcohol is oxidised to lauric aldehyde which is rapidly oxidised to lauric acid. Lauric acid is metabolised via the fatty acid and tricarboxylic acid pathways. No further details available.

**Reliability** : (2) valid with restrictions
Peer reviewed summary data on the evaluation of the metabolism of various aliphatic alcohols including Lauryl alcohol

25.11.2004 (28)

## 5.1.1 ACUTE ORAL TOXICITY

**Type** : LD50

| | | |
|---|---|---|
| **Species** | : | rat |
| **Strain** | : | other: Holzman albino |
| **Sex** | : | male/female |
| **Number of animals** | : | 10 |
| **Vehicle** | : | other: undiluted |
| **Value** | : | > 26530 mg/kg bw |
| **Method** | : | other: standard in house procedure |
| **Year** | : | 1965 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Alfol 12 |
| **Test condition** | : | TEST ORGANISMS: rat<br>- Source: not reported<br>- Weight at study initiation: 210-265 g<br>- Group size: 5M+5F<br>- Controls: no<br><br>ADMINISTRATION:<br>- Doses: 4.72, 6.66, 9.42, 13.30, 18.78 and 26.53 g/kg<br>- Doses per time period: single dose fasted overnight<br>- Volume administered or concentration: undiluted<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Observed for gross toxic effects several times on the day of dosing and daily thereafter for 14 days. Animals which died were necropsied. All survivors were weighed and necropsied at the end of the observation period. |
| **Result** | : | MORTALITY: There were no mortalities at any dose level.<br><br>CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed at any dose level on the day of dosing. Within 24 hours, diuresis was evident at all test levels. Weakness and bloody nasal discharge were exhibited by most of the animals at the top dose level (26.53 g/kg) at this time. These effects persisted for less than 72 hours. Hair loss of the posterior ventral surface of the body occurred in most of the animals at the two highest dosage levels at varying times throughout the observation period. Final weight records showed normal gain in all animals.<br><br>NECROPSY FINDINGS: Gross necropsy revealed no visceral abnormalities.<br><br>POTENTIAL TARGET ORGANS: None identified<br><br>SEX-SPECIFIC DIFFERENCES: None obvious from the report. |
| **Conclusion** | : | The rat oral LD50 for Alfol 12 was >26.53 g/kg with no obvious target organ identified. |
| **Reliability** | : | (2) valid with restrictions<br>Study well documented, meets generally accepted scientific principles, acceptable for assessment. |
| **Source** | : | Scientific Associates Inc. 1965d<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |

11.08.2005 (22)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | rat |
| **Strain** | : | Wistar |
| **Sex** | : | male/female |

| | | |
|---|---|---|
| **Number of animals** | : | 10 |
| **Vehicle** | : | other: aqueous suspension |
| **Value** | : | > 5000 mg/kg bw |
| **Method** | : | other: OECD 401 (limit dose) |
| **Year** | : | 1981 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Lorol 12 |
| **Test condition** | : | TEST ORGANISMS: Rat (Wistar)<br>- Source: Winkelmann, Hanover Germany<br>- Weight at study initiation: males mean weight 156 g, females 136 g<br>- Group size: 5M+5F<br>- Controls: no<br><br>ADMINISTRATION: gavage animals fasted<br>- Doses: 5 g/kg<br>- Doses per time period: single<br>- Volume administered or concentration: 20 ml/kg of a 25% aqueous suspension.<br>- Post dose observation period: 14 days<br><br>EXAMINATIONS: Clinical signs were observed at 1, 4 and 24 hours after dosing and then daily thoughout the obsrvation period. Body weights were recorded immediately prior to dosing and at 24 hours, 1 week and two weeks after dosing. All survivors were subject to gross necropsy. |
| **Result** | : | MORTALITY: There were no deaths during the course of the study.<br><br>CLINICAL SIGNS: Slight sedation and piloerection in all test animals during the first 24 hours after dosing. The animals gained in bodyweight at all measurement points during the observation period.<br><br>NECROPSY FINDINGS: Nothing remarkable.<br><br>POTENTIAL TARGET ORGANS: None identified<br><br>SEX-SPECIFIC DIFFERENCES: None. |
| **Conclusion** | : | The rat oral LD50 for Lorol 12 applied as an aqueous suspension was >5 g/kg. Signs of intoxication were confined to mild sedation and piloerection on the day of dosing. There were no gross histopathological changes and no evidence of specific target organ toxicity. |
| **Reliability** | : | (2) valid with restrictions<br>Guideline study |
| **Source** | : | Henkel KGaA 1981b<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |

11.08.2005 (12)

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | other: rat, rabbit |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Value** | : | > 10000 mg/kg bw |
| **Method** | : | |

| | | |
|---|---|---|
| **Year** | : | |
| **GLP** | : | |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The results from two acute oral studies are reported in Clayton and Clayton. The acute oral LD50 in rats is reported to be greater than 10.6 g/kg and 12.8 g/kg, and greater than 29.9 g/kg for rabbits. The animals that survived either 12.8 or 29.9 g/kg technical lauryl alcohol demonstrated no significant gross or microscopic changes. |
| **Reliability** | : | (4) not assignable<br>Secondary literature reference |

11.08.2005 (7)

### 5.1.2 ACUTE INHALATION TOXICITY

| | | |
|---|---|---|
| **Type** | : | LC50 |
| **Species** | : | rat |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | |
| **Vehicle** | : | |
| **Exposure time** | : | 6 hour(s) |
| **Value** | : | > 1.05 mg/l |
| **Method** | : | other: no data |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Test substance dispersed as an aerosol. This is a secondary reference with no experimental detail. |
| **Reliability** | : | (4) not assignable<br>Secondary literature |
| **Source** | : | Clayton and Clayton 1994<br>Hayes Consultancy Service Bromley, Kent |

03.09.2004 (7)

### 5.1.3 ACUTE DERMAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 8000 - 12000 mg/kg bw |
| **Species** | : | rabbit |
| **Strain** | : | New Zealand white |
| **Sex** | : | male/female |
| **Number of animals** | : | 4 |
| **Vehicle** | : | other: undiluted |
| **Doses** | : | 0.5, 1, 2, 4, 6, 8 and 12 g/kg |
| **Method** | : | other: contract laboratory protocol |
| **Year** | : | 1977 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Alfol 12 |
| **Test condition** | : | TEST ORGANISMS: Rabbit (New Zealand White) |

- Source: not reported
- Age: not reported
- Weight at study initiation: 2.28 - 3.04 kg
- Group size: low dose and high dose 2M+2F
- Controls: none

ADMINISTRATION: 24 hour application to intact and abraded skin
- Area covered: the dose was applied to the trunk of the animals under occlusion.
- Occlusion: plastic binder
- Vehicle: Applied undiluted.
- Total volume applied: maximum dose 11-12 ml/kg
- Doses: 0.5, 1, 2, 4, 8 and 12 g/kg
- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels. An estimate was made of the the amount of unabsorbed material.

EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy.

**Result** **:** MORTALITY:
- Time of death: All deaths occurred between days 2 and 10 after administration.
- Number of deaths at each dose: Intact skin 0/2, 0/2, 2/2, 1/2, 1/2, abraded skin 0/2, 1/2, 0/2,0/2, 1/2, 1/2. Combined 0/4, 1/4, 2/4, 1/4, 2/4, 2/4. It appeared that most of the test substance was absorbed.

LD50(s): The LD50 for combined abraded and intact skin was considered to be between 8 and 12 g/kg. The small group size and erratic dose response precluded separate estimation for intact and abraded skin.

APPLICATION SITE: At the end of the exposure period all animals showed slight to moderate erythema at the application site. In all survivors wrinkling and/or coreaceousness, hardening and desquamation of the skin occurred and persisted in varying degrees until the end of the observation period.

CLINICAL SIGNS: Generalised weakness and/or unthriftiness preceded death in each animal. Similar effects but to a lesser degree were observed in some survivors. 11/16 survivors appeared normal witin 96 dose of exposure. Final body weights of surviving animals showed slight to moderate loss in 8 animals, constant weight in 2 animals, and gains within expected limits in 6 animals.

NECROPSY FINDINGS: Animals which died showed one or more of the following: depletion of visceral fatty tissue, moderate accumulation of clear fluid within the peritoneal cavity, moderate congestion of lungs and kidneys, haemorrhaging and/or blanching with erosion of the gastric mucosa.

Rabbits surviving to 14 days showed slight to moderate accumulation of clearr viscous liquid within the peritoneal cavity and/or depletion of visceral fatty tissues. 9/16 rabbits showed no gross systemic changes.

POTENTIAL TARGET ORGANS: Gastric mucosa.

SEX-SPECIFIC DIFFERENCES: More females than males succumbed to the effects of the test material.

| | | |
|---|---|---|
| **Conclusion** | : | The rat dermal LD50 for this sample of Alfol 12 was in the range of 8000-12000 mg/kg (24 occluded exposure). All test animals developed skin irritation at the application site persisting throughout the observation period. Clinical signs of toxicity were generalised weakness and unthriftiness. Haemorrhage and/or blanching with erosion of the gastric mucosa was reported in premature decedents but not in rabbits which survived to the end of the exposure period. |
| **Reliability** | : | (2) valid with restrictions<br>Study well documented, meets generally accepted scientific principles, acceptable for assessment. |
| **Source** | : | Scientific Associates, Inc. 1977f<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |
| 11.08.2005 | | (24) |
| **Type** | : | LD50 |
| **Value** | : | = 1500 - 2000 mg/kg bw |
| **Species** | : | rabbit |
| **Strain** | : | New Zealand white |
| **Sex** | : | male/female |
| **Number of animals** | : | 4 |
| **Vehicle** | : | other: applied undiluted |
| **Doses** | : | 1, 1.5 and 2 g/kg |
| **Method** | : | other: contract laboratory protocol |
| **Year** | : | 1975 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Alfol 12 |
| **Test condition** | : | TEST ORGANISMS: Rabbit (New Zealand White)<br>- Source: not reported<br>- Age: not reported<br>- Weight at study initiation: 2.2 - 3.1 kg<br>- Group size: 2M+2F<br>- Controls: none<br><br>ADMINISTRATION: 24 hour application to intact and abraded skin<br>- Area covered: the dose was applied to the trunk of the animals under occlusion.<br>- Occlusion: plastic binder<br>- Vehicle: Applied undiluted.<br>- Total volume applied: maximum dose 1-2 ml/kg<br>- Doses: 1, 1.5 and 2 g/kg<br>- Removal of test substance: Excess material was washed away and the area dried with absorbent paper towels.<br><br>EXAMINATIONS: Mortality, clinical signs of systemic toxicity and skin reactions at the application site were recorded on the day of dosing and throughout the 14 day observation period. Body weights were recorded prior to dosing and on observation day 14. All decedents and survivors were subject to gross necropsy. |
| **Result** | : | MORTALITY:<br>- Time of death: All deaths occurred within 3 days of exposure. |

- Number of deaths at each dose: Intact skin 0/2, 1/2 and 2/2, abraded skin 0/2, 0/2 and 2/2.

LD50(s): Intact skin: 1.5 g/kg; Abraded skin: 1.5 - 2 g/kg; combined intact and abraded 1.5 - 2 g/kg. At the end of the 24 hour exposure period it appeared that some absorption of test material had occurred.

APPLICATION SITE: Animals at all dose levels showed erythema, wrinkling and desquamation of the application site.

CLINICAL SIGNS: At ta dose of 1g/kg there were no signs of toxicity. At higher dose levels some prostration was noted. Survivors appeared normal 72 hours after exposure. Survivors generally gained weight within expected limits with 2 exceptions one intact male at 1 g/lg sowed a slight weight loss and one abraded male at 1.5 showed a constant weight.

NECROPSY FINDINGS: In premature decedents there was some general deterioration but no dose-related lesions. Tissues of survivors sacrificed at the end of the observation period were unremarkable.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: The experimental data was reported in combined form.

**Conclusion** : The rabbit dermal LD50 of Alfol 12 was between 1500 and 2000 mg/kg. All rabbits showed irritation of the application site immediately following exposure. Some prostration was observed in animals at the higher dose levels. Necropsy findings showed no treatment related lesions.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Scientific Associates, Inc. 1975
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
11.08.2005 (23)

**Type** : LD50
**Value** : > 8310 mg/kg bw
**Species** : guinea pig
**Strain** :
**Sex** :
**Number of animals** :
**Vehicle** :
**Doses** :
**Method** : other: not specified
**Year** :
**GLP** : no data
**Test substance** : other TS: Dodecanol (112-53-8)

**Remark** : Secondary reference, limited data this was a personal communication provided by Fassett for the 1963 edition of Patty.

**Reliability** : (2) valid with restrictions

**Source** : Clayton and Clayton 1994

Hayes Consultancy Service Bromley, Kent

03.09.2004 (6)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

| | | |
|---|---|---|
| **Remark** | : | Not required OECD or HPV endpoint. |
| **Source** | : | The Weinberg Group Inc. Washington D.C<br>Shell Chemicals Ltd. London<br>Hayes Consultancy Service Bromley, Kent |

07.03.2000

### 5.2.1 SKIN IRRITATION

| | | |
|---|---|---|
| **Species** | : | other: New Zealand White rabbit |
| **Concentration** | : | |
| **Exposure** | : | Semiocclusive |
| **Exposure time** | : | 4 hour(s) |
| **Number of animals** | : | 3 |
| **PDII** | : | 3.5 |
| **Result** | : | moderately irritating |
| **EC classification** | : | irritating |
| **Method** | : | OECD Guide-line 404 "Acute Dermal Irritation/Corrosion" |
| **Year** | : | 1996 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Kalcol 2098 |
| **Test condition** | : | TEST ANIMALS: Rabbits<br>- Strain: New Zealand White<br>- Sex: Male<br>- Source: David Percival Ltd, Cheshire, UK<br>- Age: 12-16 weeks<br>- Weight at study initiation: 2.44-2.67 kg<br>- Number of animals: 3<br>- Controls: Not reported<br><br>ADMINISTRATION/EXPOSURE<br>- Preparation of test substance: The test substance was a white crystalline solid which was warmed to 40C before application.<br>- Area of exposure: 2.5x2.5 cm<br>- Occlusion: semi-occlusive<br>- Vehicle: None applied undiluted<br>- Total volume applied: 0.5 ml<br>- Exposure period: 4 hours<br>- Postexposure period: 14 days<br>- Removal of test substance: Swabbing with cotton wool soaked in 74% methylated spirits.<br><br>EXAMINATIONS<br>- Scoring system: Draize<br>- Examination time points: 1, 24, 48 and 72 hours after patch removal and at 7 and 14 days. |
| **Result** | : | AVERAGE SCORE<br>- Erythema: Individual 24+48+72 hour scores were 2 for each animal. |

Group mean 24+48+72 hour score 2. The reaction extended beyond the treatment site.
- Oedema: Individual 24+48+72 hour scores were 1.7 for each animal. Group mean 24+48+72 hour score 1.7.

The PII was 3.5 (moderately irritating)

REVERSIBILITY: Crust formation in all test animals at 7 days prevented the accurate evaluation of erythema. There was no oedema. By 14 days all erythema scores were 0.

OTHER EFFECTS: Slight desquamation was noted in all animals at 14 days.

**Conclusion** : Following a 4 hour semi-occlusive application to rabbit skin Kalcohl 2098 was a skin irritant accordng to EU criteria (group mean 24+48+72 hour score 2). Based on erythema and oedema scores Kalcohl 2098 is a mild irritant (category 3) under GHS criteria.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Sanders 1996a
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (19)

**Species** : rabbit
**Concentration** : 10 % active substance
**Exposure** : Semiocclusive
**Exposure time** : 4 hour(s)
**Number of animals** : 3
**PDII** : 1.3
**Result** : not irritating
**EC classification** : not irritating
**Method** : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year** : 1997
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Kalcol 2098

**Test condition** : TEST ANIMALS: Rabbits
- Strain: New Zealand White
- Sex: Male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.71-2.90 kg
- Number of animals: 3
- Controls: Not reported

ADMINISTRATION/EXPOSURE
- Preparation of test substance: The test substance was a white crystalline solid which was prepared as a 10% solution in PEG 400
- Area of exposure: 2.5x2.5 cm
- Occlusion: semi-occlusive
- Vehicle: polyethylene glycol 400.
- Total volume applied: 0.5 ml
- Exposure period: 4 hours
- Postexposure period: 14 days
- Removal of test substance: Swabbing with cotton wool soaked in distilled

water.

EXAMINATIONS
- Scoring system: Draize
- Examination time points: 1, 24, 48 and 72 hours after patch removal and at 7 and 14 days.

**Result** : AVERAGE SCORE
- Erythema: Individual mean 24+48+73 hour scores 0, 1.3, 1.7. Group mean 24+48+72 hour score 1.
- Edema: Individual mean 24+48+73 hour scores 0, 0.3, 0.7. Group mean 24+48+72 hour score 0.3.

REVERSIBILITY: All scores were 0 at 7 days and all test sites appeared normal at 14 days.

OTHER EFFECTS: The erythema extended beyond the test site in 2 rabbits at 24 and 48 hours. Desquamation (moderate) was observed in one of these rabbits at 7 days.

**Conclusion** : Following a 4 hour semi-occlusive exposure to rabbit skin a 10% solution of Kalcol 2098 in PEG 400 would not be considered irritant by either EU or GHS criteria. The group mean 24+48+72 hour scores for erythema and oedema were 1 and 0.3 respectively. The individual 24+48+72 hour scores did not exceed 1.5 in more than one rabbit.

**Reliability** : (1) valid without restriction
Guideline study
**Source** : Hempstock, 1997a
**Flag** : Critical study for SIDS endpoint
11.08.2005 (10)

**Species** : human
**Concentration** : undiluted
**Exposure** : Semiocclusive
**Exposure time** : 4 hour(s)
**Number of animals** : 20
**PDII** :
**Result** : not irritating
**EC classification** : not irritating
**Method** : other: patch test baed on OECD 404
**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Lorol C12-98

**Test condition** : The effect on human skin was investigated:
15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.

Study was performed under Good Clinical Practice (GCP).

**Result** : No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test).

| | | |
|---|---|---|
| **Conclusion** | : | Undiluted Lorol C12-98 did not produce any skin irritation in human vounteers following a 4 hour semi-occlusive exposure in a test based on OECD 404. |
| **Reliability** | : | (1) valid without restriction<br>Test procedure in accordance with generally accepted scientific standards and described in sufficient detail. |

25.10.2005 (11)

| | | |
|---|---|---|
| **Species** | : | human |
| **Concentration** | : | undiluted |
| **Exposure** | : | Open |
| **Exposure time** | : | 1 hour(s) |
| **Number of animals** | : | 20 |
| **PDII** | : | |
| **Result** | : | not irritating |
| **EC classification** | : | not irritating |
| **Method** | : | other: Burckhardt test, open epicutaneous |
| **Year** | : | 1996 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Lorol C12-98 |
| **Test condition** | : | The effect on human skin was investigated:<br>15 drops/plaster of undiluted test substance were added to a semi-occlusive plaster (diameter: 1.5 cm) and applied for 4 hours to the backs of healthy volunteers. Readings of erythema, edema, scaling and fissures were taken 1, 24, 48 and 72 hours after application. 20 male and female volunteers were tested. Age was 22 - 53 years with an average of 34.9 years.<br><br>Study was performed under Good Clinical Practice (GCP). |
| **Result** | : | No irritation was observed following application to the human skin of undiluted test substance for 4 hours (patch test). |
| **Conclusion** | : | Lorol C12-98 was not irritating to human skin following repeated application to non-occluded skin over a period of 1 hour. |
| **Reliability** | : | (1) valid without restriction<br>Test procedure in accordance with generally accepted scientific standards and described in sufficient detail. |

25.10.2005 (14)

### 5.2.2 EYE IRRITATION

| | | |
|---|---|---|
| **Species** | : | other: New Zealand White rabbit |
| **Concentration** | : | undiluted |
| **Dose** | : | .1 ml |
| **Exposure Time** | : | |
| **Comment** | : | not rinsed |
| **Number of animals** | : | 3 |
| **Result** | : | not irritating |
| **EC classification** | : | not irritating |
| **Method** | : | OECD Guide-line 405 "Acute Eye Irritation/Corrosion" |
| **Year** | : | 1996 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : Tradename Kalcol 2098

**Test condition** : TEST ANIMALS: Rabbit
- Strain: New Zealand White
- Sex: male
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.5-2.87 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and was warmed in a warming bath to 40C prior to instillation.
- Amount of substance instilled: 0.1 ml
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize adn modifies Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

**Result** : AVERAGE SCORE (24+48+72 hour)
- Cornea: All 0
- Iris: All 0
- Conjunctivae (Redness): Individual scores 2 rabbits 0 the remaining rabbit 0.3. (group mean score 0.1)
- Conjunctivae (Chemosis): All 0
- Overall irritation score: maximum group mean score of 8.7. Classified as a minimal eye irritant according to Kay & Callandra (modified).

DESCRIPTION OF LESIONS: No corneal or iridial effects were noted suring the study. Moderate conjunctival irritation was noted in two treated eyes with minimal conjunctival irritation in the remaining treated eye one hour after treatment. Minimal conjunctival redness was noted in one treated eye at the 24 hour observation point.

REVERSIBILITY: All scores were 0 at 48 and 72 hours.

OTHER EFFECTS: Conjunctival discharge was noted in all animals one hour after instillation.

**Conclusion** : Kalcol 2098 is not irritating to the rabbit eye using either EU or GHS criteria.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Sanders 1996d
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (20)

## 5.3 SENSITIZATION

**Type** : Guinea pig maximization test

**Species** : other: Hartley albino guinea pigs

**Concentration** : Induction 3 % intracutaneous

Induction 50 % occlusive epicutaneous
Challenge 10 % occlusive epicutaneous

**Number of animals** : 10
**Vehicle** : other: liquid paraffin
**Result** : not sensitizing
**Classification** : not sensitizing
**Method** : OECD Guide-line 406 "Skin Sensitization"
**Year** : 1997
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Kalcol 2098

**Test condition** : TEST ANIMALS: Guinea pigs
- Strain: albino Hartley
- Sex: female
- Source: Japan SLC, Shizuoka
- Age: 4 weeks
- Weight at study initiation: 276-323 g
- Number of animals: 10F
- Controls: 5F

ADMINISTRATION/EXPOSURE
- Study type: adjuvant, maximization test
- Preparation of test substance for induction: In liquid paraffin
- Preparation of test substance for induction: In liquid paraffin
- Induction schedule: Single intradermal injection followed 7 days later by a 48 hour occlusive patch applied topically.
- Concentrations used for induction: 3% intracutaneous, 50% topical
- Concentration in Freuds Complete Adjuvant (FCA): 1:1 water in oil emulsion of 6% test substance in FCA and saline.
- Challenge schedule: 21 days after first induction topical application of an occluded patch for 24 hours.
- Concentrations used for challenge: 3 and 10%
- Rechallenge: No
- Positive control: DNCB and formalin, not concurrent evidence presented over a relevant time period that the strain of guinea pig did respond to known sensitisers.

EXAMINATIONS
- Grading system: 0 = no visible change, 1 = discrete or patch erythema; 2 = moderate and confluent erythema; 3 = intense erythema and swelling.
- Pilot study: Using 4 animals and multiple patches Kalcol 2978 was tested at concentrations from 0.1% - 10% intradermally and at 10, 30 and 100% topically.

**Result** : RESULTS OF PILOT STUDY: Following intradermal injection significant skin irritation was seen at concentrations of 5 and 10% persisting for 72 hours. The 3% concentration showed evidence of irritation at 24 hours only. Following topical application the undiluted material was irritant up to 48 hours, 2/4 guineapigs showed irritation at 10% while there was no evidence of irritation with the 3% concentration.

RESULTS OF TEST
- Sensitization reaction: There was no evidence of sensitisation in any of the test animals. Reactions at 24 and 48 hours following challenge with the solvent control (liquid paraffin) and 3% and 10% solutions were 0/10 treated, 0/5 control.
- Clinical signs: There were no significant differences in general condition and body weight gain between test and control groups over the course of

the test.
- Rechallenge: Not required.

**Conclusion** : Kalcol 2078 is not a skin sensitiser when tested according to the M&K maximisation procedure.

**Reliability** : (1) valid without restriction
Guideline study
**Source** : Iihama 1997a
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
07.12.2005 (15)

## 5.4 REPEATED DOSE TOXICITY

**Species** : rat
**Sex** : male/female
**Strain** : Wistar
**Route of admin.** : oral feed
**Exposure period** : Males 41-45 days; Females aprox. 54 days
**Frequency of treatment** : continuous in the diet
**Post obs. period** : none
**Doses** : 0, 1500, 7500 & 30,000 ppm (approx 100, 500, 2000 mg/kg bw/day)
**Control group** : yes
**NOAEL** : = 2000 mg/kg bw
**Method** : other: Draft OECD 422 Combined Repeat dose and Reproductive/Developmental Toxicity Screening Test.
**Year** : 1992
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS
- Age: 7 weeks
- Number of animals: 12M+12F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: males: 41-44 days; females approx. 54 days
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet. Diet preparation involved first mixing an aqueous dodecanol solution with the barley component, which varied for each dose level. The other components of the diet were then added.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality: Daily
- Body weight: weekly
- Food consumption: weekly
- Water consumption: ad lib
- Haematology: Males only at day 37; haematocrit, Hb, total RBC & WBC and differential WBC. No indication as to whether animals were fasted prior to sampling.
- Biochemistry: Males only at day 37; Plasma protein, alkaline phosphatase, AAT, glucose, urea, creatinine,total & free cholesterol and triglyceride. No indication as to whether animals were fasted prior to sampling.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):

- Macroscopic: Full necrospy on all animals.
- Organ weights: liver, kidneys, thymus (females) liver, kidney, thymus, testes, epididymes (male)
- Microscopic: Carried out on all control and top dose animals plus any obvious lesions observed at necrospy. Organs examined were liver, kidneys, adrenals, brain, heart, spleen, ovaries or testes and epididymes.

OTHER EXAMINATIONS: The results of foetal examinations and reproductive parameters are reported in the appropriate sections.

STATISTICAL METHODS: Using the SAS-stat program analysis of variance plus Dunnett's test if changes were significant.

**Result** **:** NOAEL 2000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
Males: 102.4, 530.8 and 2046.4 mg/kg/day (mean of values reported for 2 weeks prior to mating and 3 weeks after mating)
Females:130.5, 657.5 and 2870.5 mg/kg/day (mean of values reported 2 weeks prior to mating)
- Time of death: There were no mortalities in this study.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: None reported
- Body weight gain: No differences between treated and controls of either sex.
- Food consumption/food efficiency: No differences between treated and controls of both sexes.
- Clinical chemistry: (males only investigated) There was a significant reduction in plasma triglyceride (TG) at the top dose level and a significant reduction in plasma free cholesterol (F-chol) at the intermediate dose level. The reduced cholesterol level was re-analysed after removing 2 outlying values when the statistical significance was lost. These results may have been confounded by the difference in dietary composition between groups.

| | 0 | 100 | 500 | 2000 mg/kg |
|---|---|---|---|---|
| T-chol | 1.60 | 1.74 | 1.64 | 1.75 |
| F-chol | 0.18 | 0.16 | 0.11* | 0.15 |
| TG | 0.58 | 0.42 | 0.45 | 0.31** |

* P<0.05 ** P<0.01 T-chol Total cholesterol

- Haematology: (males only investigated) A dose related reduction in total WBC was observed which reached statistical significance in top and mid dose males, there were no differences in the differential white cell count which explained these observations. The mean white blood cell counts (mmol/l) for males were at 0, 100, 500 and 2000 mg/kg 7.0, 5.9, 4.3*** and 4.7** respectively. ** P<0.01 *** P<0.001

- Organ weights: There were no dose related changes in organ weights. In males only there was a reduction in relative and absolute liver weights at the low dose level and a reduction in relative liver weight at mid doses, the top dose was comparable to controls.

| | 0 | 100 | 500 | 2000 mg/kg |
|---|---|---|---|---|
| Abs liver wt | 12.27 | 11.20* | 11.76 | 11.98 |
| Rel. liver wt | 3.3 | 3.1* | 3.1* | 3.3 |

* P<0.05

- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological changes.

STATISTICAL RESULTS: reported above.

**Conclusion** : The NOAEL for systemic toxicity in male rats is considered to be 2000 mg/kg/day (highest dose tested) in the absence of toxicologically significant effects at any dose level. A reduction in white cell count in all treatment groups was considered of doubtful significance in the absence of any changes in the differential cell count (based on WBC the NOEL is <100 mg/kg/day). A reduction in triglyceride and cholesterol levels at the top dose level, while possibly indicative of mild liver effects, may have been confounded by differences in dietary composition.

**Reliability** : (2) valid with restrictions
Comparable to guideline study (draft guideline) with acceptable restrictions

**Source** : Hansen 1992a
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

09.01.2006 (9)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : other: Bacterial reverse mutation assay (Ames Test)
**System of testing** : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
**Concentration** : 4, 20, 100, 500 and 2500 ug per plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: Henkel-method "Salmonella typhimurium reverse mutation assay" (comparable to OECD Guideline 471)
**Year** : 1982
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Lorol 12

**Test condition** : METHOD Bacterial reverse mutation assay based on OECD 471. Full experimental details were not provided but actual results were available. 2-aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Four per dose level.
- Application: Plate incorporation.

- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain tested. Positive controls gave an appropriate increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: Total inhibition of bacterial growth at 2500 ug/plate for all strains tested except TA100 and at 500 ug/plate for TA1535 and 1537. Growth inhibition observed in TA100 at 2500 ug/plate and in all other strains at 100 or 500/plate.
- Without metabolic activation: Total inhibition of bacterial growth at 2500 and 500 ug/plate some inhibition at 100 ug/plate.

**Conclusion** : The C12 alcohol Lorol C12 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Cytotoxicity evidenced by complete or partial growth inhibition was observed at concentrations of >= 100 ug/plate.

**Reliability** : (2) valid with restrictions
Limited documentation, in house method acceptable for assessment
**Source** : Henkel KGaA 1982b
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
11.08.2005 (13)

**Type** : other: Bacterial reverse mutation assay (Ames Test)
**System of testing** : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538 and E. coli WP2uvrA
**Concentration** : 0.01 to 50 ug/plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: modified Ames test
**Year** : 1985
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : METHOD Modified Ames test.

SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, TA 1538 and Escherichia coli strain WP2uvrA
- Deficiences/Proficiences: Salmonella typhimurium strains histidine deficient, E. coli tryptophan deficient.
- Metabolic activation system: Rat liver S9 induced with the PCB KC 500.

ADMINISTRATION:
- Dosing: 0.01, 0.05, 0.1, 0.5, 1, 5, 10 and 50 ug/plate.
- Number of replicates: Duplicates.
- Application: Preincubation method, vehicle DMSO.

- Positive and negative control groups and treatment: Negative control DMSO. Postitive controls as appropriate 2-(2-furyl)-3-(5-nitro-2-furyl) acrylamide 0.01 or 0.05 ug/plate; N-ethyl-N'-nitro-N-nitrosoguanidine 5 ug/plate; 9-aminoacridine 80 ug/plate; 4-nitroquinoline-1-oxide 0.25 ug/plate; benzo[a]pyrene 5 ug/plate; 2-aminoanthracene 5 ug/plate;
- Pre-incubation time: 20 minutes at 37C
- Incubation time: 48hours at 37C

CRITERIA FOR EVALUATING RESULTS: Not reported.

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any of the test organisms. Positive controls produced appropriate increases in mutation rate.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With metabolic activation: >50 ug/plate (highest dose leve tested)
- Without metabolic activation: E. coli WP2 uvrA > 50 ug/plate; TA1535 10 ug/plate; other strains 50 ug/plate evidenced by growth inhibition.

**Conclusion** : Dodecanol did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium or tryptophan dependent E.coli WP2 uvrA in the presence or absence of metabolic activation. The material was tested to cytotoxic concentrations in the absence of S9.

**Reliability** : (2) valid with restrictions
Publication reporting Ames tests on various chemicals, acceptable for assessment

**Source** : Shimizu et al. 1985.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (25)

**Type** : Bacterial reverse mutation assay
**System of testing** : Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
**Concentration** : 0.5 to 500 ug/plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : OECD Guide-line 471
**Year** : 1996
**GLP** : yes
**Test substance** : other TS: Dodecanol CAS RN 112-53-8. Kalcohl 2098.

**Test condition** : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium TA 1535, 1537, 1538, 98 and 100.
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: Based on a preliminary screening test, 0.5 (only TA1538 and 1537), 1.5, 5, 15, 50, 150 and 500 (only TA98, 100, 1535) ug/plate.
- Number of replicates: triplicates
- Application: pLate incorporation, vehicle DMSO.
- Positive and negative control groups and treatment: Negative control -

vehicle (DMSO) Positive controls N-ethyl-N'-nitro-N-nitrosoguanidine 3 ug/plate (TA100) or 5ug/plate (TA1535); 9-aminoacridine 80 ug/plate (TA1537); 4-nitro-o-phenylene daimine 5 ug/plate (TA1538); 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98); 2-aminoanthracene 1ug/plate TA100, 2 ug/plate (TA1535 and TA 1537), 0.5 ug/plate (TA1538 and TA98).
- Incubation: 48 hours at 37C.

DESCRIPTION OF FOLLOW UP REPEAT STUDY: Additional dose levels were tested as follows: Without S9 0.5, 1.5, 5, 15, 50 and 150 ug/plate With S9 0.5, 1.5, 5, 15, 50, 150, 500 and 1500 ug/plate. Strains TA100 and TA1538 were not tested at the two highest dose levels. The tested was replicated with extra dose levels to allow for the cytotoxicity of the test material.

CRITERIA FOR EVALUATING RESULTS: Considered positive if there is dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub toxic dose levels. To be considered negative the number of induced revertants should be <2 fold the number of spontaneous revertants and dose levels should extend to the limits of solubility or toxicity up to a maximum fo 5000 ug/plate.

STATISTICAL METHOD(S); Dunnetts linear regression method.

**Result** : GENOTOXIC EFFECTS:
With and without metabolic activation: No increase in reverse mutation rates at any test concentration. All positive and negative controls showed an appropriate response.

PRECIPITATION CONCENTRATION: An oily precipitate was observed at and above 1500 ug/plate in the preliminary toxicity assay, this did not interfere with the scoring of revertant colonies and was not reported when this dose level was tested in the repeat study.

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: The test material exhibited a visible reduction in background lawn at and above 150 ug/plate in all the strains tested. Strains TA1538, 1537 and 1535 also showed a reduction in background lawn at 50 ug/plate. This indicates that the material was tested to a toxic level.

STATISTICAL RESULTS: No statistically significant increase in reverse mutation rate at any dose level tested with or without metabolic activation.

**Conclusion** : The C12 alcohol Kalcohl 2098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation. The material was tested to cytotoxic concentrations.

**Reliability** : (1) valid without restriction
**Source** : Thompson 1996a
**Flag** : Critical study for SIDS endpoint
27.11.2003 (29)

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Micronucleus assay
**Species** : mouse

| | | |
|---|---|---|
| **Sex** | : | male/female |
| **Strain** | : | other: albino mice, CFW 1 |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 24, 48, 72 hours |
| **Doses** | : | 5000 mg/kg bw |
| **Result** | : | negative |
| **Method** | : | OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test" |
| **Year** | : | 1992 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Lorol 12 |
| **Test condition** | : | TEST ORGANISMS: Mouse CFW 1<br>- Age: 7-8 weeks<br>- Weight at study initiation: males 21-27g, females 21-26g<br>- No. of animals per dose: 6M + 6F<br><br>ADMINISTRATION:<br>- Vehicle: Arachis oil.<br>- Duration of test: 1 day, single administration.<br>- Frequency of treatment: Once.<br>- Sampling times and number of samples: 24, 48 and 72 hours after treatment. Two slides were prepared for each animal and 1000 polychromatic erythrocytes (PCE) scored.<br>- Control groups and treatment: Solvent control arachis oil, 10 ml/kg: positive control cyclophosphamide, 20 mg/kg; test substance 1-dodecanol 5000 mg/kg (dose volume 10 ml/kg)<br><br>EXAMINATIONS:<br>- Clinical observations: Daily<br>- Organs examined at necropsy: None.<br>- Criteria for evaluating results: A statistically significant ($p<0.05$) increase in PCE compared to controls. Method used Kastenbaum & Bowman.<br>- Criteria for selection of M.T.D.: Based on a screening test. Effects seen at 5000 mg/kg were piloerection only. |
| **Result** | : | MORTALITY: None<br><br>CLINICAL SIGNS: Piloerection in all test animals.<br><br>NECROPSY FINDINGS: Not reported.<br><br>BODY WEIGHT CHANGES: Not reported.<br><br>FOOD AND WATER CONSUMPTION CHANGES: Not reported.<br><br>PCE/NCE RATIO: There was no effect on this ratio.<br><br>GENOTOXIC EFFECTS: There was no increase in the incidence of micronucleated cells in the test group. The incidence of micronuclei in the contorl group was within historical control ranges. The positive control group produced an appropriate increase in numbers of micronucleated cells.<br><br>STATISTICAL RESULTS: No statistically significant increase in micronucleated polychromatic erythrocytes compared to vehicle controls, the positive control group did produce a statistically significant increase. |
| **Conclusion** | : | Lorol 12 did not increase the % of micronucleated erythrocytes or the |

PCE:NCE ratio in mice at any time interval after treatment (24, 48 or 72 hours) at dose levels up to 5000 mg/kg bw when compared to vehicle controls.

**Reliability** : (1) valid without restriction
Guideline study
**Source** : Banduhn, 1992
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
11.08.2005 (3)

## 5.7 CARCINOGENITY

**Species** : mouse
**Sex** : no data
**Strain** : other: C3H/He
**Route of admin.** : dermal
**Exposure period** : 100 weeks
**Frequency of treatment** : twice weekly
**Post. obs. period** : none
**Doses** : see below
**Result** : negative
**Control group** : yes
**Method** : other: investigation of cocarcinogenic activity
**Year** : 1969
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS
- Number of animals: mice (sex unspecified) 20/group treated, controls 50.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 100 weeks
- Type of exposure: dermal, twice weekly
- Post exposure period: none
- Vehicle: Decalin/dodecanol
- Total volume applied: 50 mg/mouse
- Doses: Carcinogen benzo[a]pyrene at a concentration of either 0.05 or 0.2% in a mixture of decalin and dodecanol containing concentrations of dodecanol ranging from 0-100%. A control group received a 50:50 mixture of decalin/ dodecanol.

OBSERVATIONS: The incidence of skin tumours was recorded over the 100 week time period. There was no report of the degree of skin irritation at the application site during the exposure period.

**Result** : There were no skin tumors seen in the 50 control animals receiving 50% dodecanol in decalin alone.

In mice receiving benzo[a]pyrene [BaP] in a mixture of decalin and dodecanol the latent period for skin tumour development decreased with increasing concentrations of dodecanol. The latent period for development of BaP (0.2%) intitiated skin tumours was 42 weeks in decalin alone and 22 weeks with dodecanol alone. At the lower dose level of BaP (0.05%) the difference was greater with a latent period of 63 weeks reduced to 26 weeks.

**Conclusion** : Dodecanol was not a skin carcinogen when applied topically to the skin of

mice twice weekly for 100 weeks as a 50:50 mixture with decalin. When applied with BaP dodecanol reduced the latent period for development of BaP initiated skin tumours in a dose related manner.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.
**Source** : Bingham and Falk 1969.

Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
11.08.2005 (4)

**Species** : mouse
**Sex** : female
**Strain** : other: ICR/Ha Swiss
**Route of admin.** : dermal
**Exposure period** : 440 days
**Frequency of treatment** : three times per week
**Post. obs. period** : none
**Doses** : 10 mg dodecanol
**Result** : negative
**Control group** : yes
**Method** : other: investigation of cocarcinogenicity
**Year** : 1976
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS Mouse ICR/Ha swiss females only.
- Age: 6-8 weeks
- Weight at study initiation: Not reported
- Number of animals: 50 per group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 440 days
- Type of exposure: dermal thrice weekly application to the shorn dorsal skin.
- Post exposure period: none
- Vehicle: Acetone
- Concentration in vehicle: Not reported
- Total volume applied: 0.1 ml
- Doses: Carcinogenesis experiment 10 mg dodecanol in acetone; Cocarcinogenesis experiment 10 mg dodecanol + 5 ug benzo[a]pyrene in acetone. Vehicle, untreated and positive controls were included. Anthralin and PMA were ositive controls for cocarcinogenesis, BaP (5 ug in 0.1 ml solvent) the carcinogenesis control. The dose levels were chosen on the basis of range findng tests carried out over a period of 2-4 weeks and were the highest doses at which skin irritation was minimal.

CLINICAL OBSERVATIONS AND FREQUENCY
The animals were observed regularly (no more specific details). Tumours were recorded and those >1mm in diameter were counted and charted regularly. Only tumours persisting for >=30 days were counted in the cumulative totals. There was no report of the degree of skin irritation at the application site during the exposure period.
- Macroscopic examination: At 440 days. Animals bearing bearing malignant skin tumours (carcinomas) were sacrificed either within 2 months of the categorisation as maligant or when they appeared moribund.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
All animals were autopsied. Specimens from tumors and any abnormal tissues were confirmed histologically.

**Result** : None of the mice exposed to the alcohol alone developed any skin tumours, neither did the untreated or vehicle control mice.

In the cocarcinogenicity experiment the incidence of skin tumours was as follows:

BaP in acetone: mice with papillomas 21, total papillomas 26, carcinomas 12, latent period (days to first papilloma) 210.

BaP + dodecanol in acetone: mice with papillomas 16, total papillomas 27, total carcinomas 13, latent period 226 days.

BaP + PMA: mice with papillomas 45, total papillomas 260, total carcinomas 37, latent period 60 days.

BaP + Anthranilin: mice with papillomas 25, total papillomas 58, total carcinomas 15, latent period 159 days.

The authors conclude that dodecanol has weak to moderate cocarcinogenic potential.

**Conclusion** : Dodecanol (lauryl alcohol) has no skin tumorigenic potential when applied to the mouse skin thrice weekly for 440 days in acetone. There was apparently some evidence of weak cocarcinogenic activity when dodecanol was administered together with BaP as evidenced by an increased incidence of skin tumours compared to mice treated with BaP alone but there was no decrease in the latent period.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Van Duuren and Goldschmidt 1976.

Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
11.08.2005 (27)

**Species** : mouse
**Sex** : female
**Strain** : Swiss
**Route of admin.** : dermal
**Exposure period** : 60 weeks
**Frequency of treatment** : three times weekly
**Post. obs. period** : none
**Doses** : 4 ug/mouse in cyclohexane
**Result** : negative
**Control group** : no
**Method** : other: skin tumour promotion study
**Year** : 1966
**GLP** : no data
**Test substance** : other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Test substance** : The substances correspond to C6 through C18 (even carbon number)

alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%.

**Test condition** : TEST ORGANISMS
- Age/weight: Not reported
- Number of animals: 30-50 female swiss mice/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 60 weeks
- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.
- Post exposure period: None
- Vehicle: cyclohexane
- Concentration in vehicle: 20%
- Total volume applied: (1 drop approx. 2ul)
- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.

The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.

OBSERVATIONS
Skin tumour development was reported and the degree of skin irritation at the application site was assessed.

**Result** : No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:

hexanol = 0/50
octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)
decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)
dodecanol = 2/30 (appeared at week 39 and 49)
tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.

**Conclusion** : In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999).

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles,

acceptable for assessment.

**Source** : Sice 1966.

Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (2) (17) (18) (26)

| | | |
|---|---|---|
| **Species** | : | mouse |
| **Sex** | : | no data |
| **Strain** | : | other: Swiss albino ddY |
| **Route of admin.** | : | i.p. |
| **Exposure period** | : | 5 days |
| **Frequency of treatment** | : | daily |
| **Post. obs. period** | : | 24 days |
| **Doses** | : | Test 1: 2.5 or 10 mg/mouse/day. Test 2: 2, 4 or 8 mg/mouse/day 2.5 and 10 mg/mouse/day for C16 & 18 alcohols. |
| **Result** | : | negative |
| **Control group** | : | yes |
| **Method** | : | other: determination of antitumour activity against Ehrlichs Ascites Tumour |
| **Year** | : | 1972 |
| **GLP** | : | no |
| **Test substance** | : | other TS: Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol |

**Test condition** :

TEST ORGANISMS Mouse Swiss albino ddY implanted ip with ascites tumour cells.
- Age: 5 weeks
- Weight at study initiation: 20-23g
- Number of animals: 4 or 6/ treatment group, 20 controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 5 days starting 24 hours afeter implantation of the ascites tumour cells.
- Type of exposure: Intraperitoneal
- Post exposure period: 24 days
- Vehicle: Probably aqueous suspension using Tween 80.
- Concentration in vehicle: Not reported.
- Doses: Test 1: for all 5 alcohols tested dose levels were 2.5 and 10 mg/mouse. Test 2: C10, 12 and 14 alcohols were tested at 2, 4 and 8 mg/mouse, C16 and 18 alcohols were tested at 2.5 and 10 mg/mouse.

OBSERVATIONS
The mean survival time was recorded and compared to the untreated control group.

**Result** : The C10, 12, and 14 alcohols exhibited toxicity to the mice, evidenced by severe diarrhoea and loss of body weight. The dose levels were reduced in the repeat test. The mean survival time for the untreated control group (Ascites implantation only) was 18.3 days in test1 and 14.4 days in test 2. All of the alkanols tested increased the survival time of mice implanted with ascites tumour cells at one or more dose levels tested. Life span was prolonged by 124 - >194%.

**Conclusion** : Treatment with C10 -18 alcohols extended the survival time of mice implanted intraperitoneally with Ehrlich ascites tumour cells.

**Reliability** : (2) valid with restrictions
Screening test acceptable for assessment

**Source** : Ando et al, 1972

Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (1)

| | | |
|---|---|---|
| **Species** | : | mouse |
| **Sex** | : | female |
| **Strain** | : | ICR |
| **Route of admin.** | : | dermal |
| **Exposure period** | : | not reported |
| **Frequency of treatment** | : | single application of the initiator 7,12-dimethylbenz[a]anthracene |
| **Post. obs. period** | : | Repeated applications of 50:50 1-octadecanol and 1-dodecanol |
| **Doses** | : | 125 ug DMBA |
| **Result** | : | |
| **Control group** | : | no data specified |
| **Method** | : | other: tumour promotion study |
| **Year** | : | 1974 |
| **GLP** | : | no |
| **Test substance** | : | other TS: 50:50 mixture of 1-octanol and 1-dodecanol |
| **Test condition** | : | A mixture of equal parts 1-octadecanol and 1-dodecanol was applied repeatedly (frequency not reported) to the skin of mice which had been initiated with a single application of the carcinogen 7,12-dimethylbenzanthracene. |
| **Result** | : | A mixture of 1-octadecanol and 1-dodecanol in equal parts exhibited weak tumour promoting activity at concentrations of 1% or more. When added to Tween 80 there was a moderate reduction in the tumour promoting activity of the Tween 80 particularly at high concentrations (actual concentrations not reported). The is no indication of the degree of irritation observed following the various applications. |
| **Conclusion** | : | This study was reported in abstract form only and is included for completeness. |
| **Reliability** | : | (4) not assignable<br>Screening test acceptable for assessment |
| **Source** | : | Bock & Tso, 1974<br>Hayes Consultancy Service Bromley, Kent |

11.08.2005 (5)

### 5.8.1 TOXICITY TO FERTILITY

| | | |
|---|---|---|
| **Type** | : | other: Combined repeat dose and Reproductive/Developmental screening study |
| **Species** | : | rat |
| **Sex** | : | male/female |
| **Strain** | : | Wistar |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | Males 41-44 days , females up to 54 days |
| **Frequency of treatment** | : | continuous in diet |
| **Premating exposure period** | | |
| **Male** | : | 14 days |
| **Female** | : | 14 days |
| **Duration of test** | : | Males 41-44 days , females up to 54 days |
| **Doses** | : | 0, 100, 500, 2000 mg/kg bw/day |
| **Control group** | : | yes |

| | | |
|---|---|---|
| **NOAEL Parental** | : | = 2000 mg/kg bw |
| **NOAEL F1 Offspr.** | : | = 2000 mg/kg bw |
| **Method** | : | other: Combined repeat dose and reproductive/developmental toxicity screening test |
| **Year** | : | 1992 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ORGANISMS: Rat Wistar aged 8 (males) - 9 (females) weeks at start of exposure period. 12M+12F/group

ADMINISTRATION / EXPOSURE
- Type of exposure: Dietary
- Duration of test/exposure: males 41-44 days, females approx. 54 days
- Treatment:
- Control group and treatment:
- Vehicle: Diet
- Concentration in vehicle: 0, 1500, 7500 & 30,000 ppm

MATING PROCEDURES: 14 day premating exposure, then 1M+1F caged together. Inspection for vaginal plugs thrice daily. If mating did not occur after 14 days cohabitation the female was placed with another male for 8 days.

STANDARDIZATION OF LITTERS: No

PARAMETERS ASSESSED DURING STUDY P:
- Clinical observations: body weight, weight gain, food consumption, food efficiency.
- Estrous cycle: Exposure was for 14 days premating covering at least 2 oestrous cycles. Ovaries were weighed and examined histopathologically at section (21 days after birth).
- Sperm examination: Exposure 14 days premating, no specific sperm analyses carried out, the testes & epididymes were weighed and examined histopathologically.
- Reproductive parameters: Pregancy rate, length of gestation, implantations, corpora lutea and resorptions were recorded.

OFFSPRING: Offspring (and dams) were sacrificed on post natal day 5 and the pups were weighed and examined for external malformations than sexed and examined for internal malformations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: liver, kidneys, thymus, testis, epididymes.
- Histopathology P: liver, kidneys, adrenals, brain, heart, spleen, ovaries, thymus, testes, epididymides and any organs showing abnormality on macroscopic examination were fixed. The above tissues from all controls and top dose treated rats (except the thymus) plus abnormalities were examined.
- Macroscopic P: Full macroscopic examination.

OTHER EXAMINATIONS: Haematological and biochemical parameters were measured for the Repeat dose toxicity assessment, full details in Chapter 5.4 Repeat dose toxcity

STATISTICAL METHODS: Analysis of variance followed if significant differences were established by Dunnetts T-test to assess possible intergroup differences. For pregnancy rate a Qui2-test was carried out to confirm lack of significance.

**Result** : NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 500 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1:
- Body weight: No treatment related effects.
- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.
- Pregancy rate: There was no statistically significant difference in pregancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 83%, 2000 mg/kg/day 75% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams (23 days in all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Effects on sperm: Not reported
- Clinical biochemistry findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Haematological findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Organ weights: There were no statistically significant dose related changes in organ weights including the testes, epididymes and ovaries.
- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological changes including no effects in the testes and ovaries.
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups (mean 13 in control group, 14 in each treated group). There were no resorptions.
- Number of corpora lutea: No significant differences between treated and control groups (mean 14 in test and controls).
- Ovarian primordial follicle counts: Not reported
- Offspring toxicity F1:
- Litter size and weights: No effect of treatment. Litter size mean Controls 13.25, low dose 13.27, mid dose 13.2, high dose 13.33. Mean litter weights at day 1 were 75, 75, 71 and 77 gm and at day 4 106, 107, 101 and 104 gm for control, low, mid and high dose respectively. No statistical significance.
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.

**Conclusion** : Parental NOAEL 2000 mg/kg/day. No adverse effects were observed on reproductive parameters and the NOAEL for reproductive and developmental effects can also be considered to be 2000 mg/kg/day.

**Reliability** : (2) valid with restrictions
Comparable to guideline study (draft guideline) with acceptable restrictions

**Source** : Hansen 1992a.
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
11.08.2005 (9)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Wistar |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | Up to 54 days, premating, mating and gestation until post natal day 5. |
| **Frequency of treatment** | : | continuous in diet |
| **Duration of test** | : | up to 54 days |
| **Doses** | : | 0, 100, 500, 2000 mg/kg bw/day |
| **Control group** | : | yes |
| **NOAEL Maternalt.** | : | = 2000 mg/kg bw |
| **NOAEL Teratogen** | : | = 2000 mg/kg bw |
| **Method** | : | other: Combined repeat dose and reproductive/developmental toxicity Screening Test |
| **Year** | : | 1992 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | other TS: Dodecanol (112-53-8) Purity >99% |
| **Test condition** | : | Groups of 12 female rats were given dodecanol in the diet at doses of 0, 1500 ppm, 7500 ppm, and 30000 ppm (0, 100, 500 and 2000 mg/kg/day) for a period of 14 days prior to mating then throughout mating and gestation until post natal day 5 when dams and offspring were sacrificed. This is part of a combined repeat dose and reproductive/ developmental screening study (guideline draft OECD 422) Reproductive parameters examined were pregancy rate, length of gestation, implantations, corpora lutea and resorptions. On post natal day 5 the pups were weighed and examined macroscopically for external malformations then sexed and examined for internal malformations. For full details of this study see chapter 5.4 Repeated dose toxicity and chapter 5.8.1 Fertility |
| **Result** | : | NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.<br><br>ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: ca 100, 500 and 2000 mg/kg/day<br><br>TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:<br>- Parental data:<br>- Body weight: No treatment related effects.<br>- Food/water consumption: No treatment related effects.<br>- Description, severity, time of onset and duration of clinical signs: None reported.<br>- Pregancy rate: There was no statistically significant difference in pregancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 83%, 2000 mg/kg/day 75% these were within the normal historical control range according to the authors (actual historical control data not presented). Lack of statistical significance confirmed using Qui2-test.<br>- Fertility index: Not reported<br>- Precoital interval: Not reported |

- Duration of gestation: Comparable in treated and control dams (23 days in all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups (mean 13 in control group, 14 in each treated group).. There were no resorptions.
- Number of corpora lutea: No significant differences between treated and control groups.
- Ovarian primordial follicle counts: Not reported
- Foetal toxicity:
- Litter size and weights: No effect of treatment. Litter size mean Controls 13.25, low dose 13.27, mid dose 13.2, high dose 13.33. Mean litter weights at day 1 were 75, 75, 71 and 77 gm and at day 4 106, 107, 101 and 104 gm for control, low, mid and high dose respectively. No statistical significance.
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.
- Foetal anomalies: There were no treatment related changes in the incidence of external or visceral malformations visible on macroscopic examination.

**Conclusion** : Development was assessed as part of a combined repeat dose and reproductive/developmental toxicity study. There were no adverse effects on maternal toxicity or reproductive parameters and no adverse effect on the offspring which were examined on postnatal day 5. The NOAEL for maternal and foetotoxicity was 2000 mg/kg/day in rats receiving dodecanol in the diet for up to 54 days (premating, mating, gestation to postnatal day 5). There was no evidence of teratogenicity from the limited examinations of the pups which were carried out.

**Reliability** : (1) valid without restriction
Comparable to guideline study (draft guideline) with acceptable restrictions

**Source** : Hansen 1992a.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
11.08.2005 (9)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

**Remark** : The purpose of this study was to compare the nitrocellulose-replica method (24 hour semi-occlusive exposure to the flexor surface of the arms) with closed patch testing (24 hour application to the back in a Finn chamber, 15 ul test material). The study was based on 20 healthy volunteers.

The results evaluated using the closed patch testing showed that skin

irritation for octanol significantly increased with increasing concentration of the test compound. Lauryl, cetyl and stearyl alcohols were of low irritancy. However the nitrocellulose-replica method could detect skin irritation with the higher alcohols which was not observed in the closed patch testing.

**Source** : Sato et al, 1996
Hayes Consultancy Service Bromley, Kent

**Test substance** : octyl alcohol, lauryl alcohol, cetyl alcohol, stearyl alcohol.

**Reliability** : (2) valid with restrictions
03.09.2004 (21)

**Remark** : The purpose of this study was to introduce the chamber-scarification test designed for increased sensitivity for assessing the irritancy of materials. It is important to note that persons especially vulnerable to irritants were selected.

The materials were applied as a 25% solution in mineral oil. The skin is first scarified and the test material applied (0.1 ml) in a test chamber once daily for 3 days to groups of 5-10 volunteers. The skin was assessed 30 minutes after the end of the final exposure.

The degree of irritatin was related to carbon chain length, the C10 and C12 alcohols giving a marked response while the C14 alcohol gave a moderate response, C16 slight and the oleyl alcohol gave a low response.

**Source** : Frosch & Kligman, 1976
Hayes Consultancy Service Bromley, Kent

**Test substance** : oleyl alchol, hexadecyl alcohol, tetradecyl alcohol, dodecyl alcohol, decyl alcohol

**Reliability** : (2) valid with restrictions
03.09.2004 (8)

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# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

Note: References in this file are given separately for physicochemical properties, environmental fate, ecotoxicology (i.e. chapters 2-4) and human health endpoints (chapter 5).

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 112-92-5 |
| **CAS No.** | **:** | 112-92-5 |
| **EINECS Name** | **:** | octadecan-1-ol |
| **EC No.** | **:** | 204-017-6 |
| **TSCA Name** | **:** | 1-Octadecanol |
| **Molecular Formula** | **:** | C18H38O |

## 2.1 Melting Point

**Value:** = 59.5 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** SRC.
**Reliability:** (4) not assignable
24-SEP-2003 (14)

**Value:** = 58 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** Lington and Bevan 1994.
**Reliability:** (4) not assignable
24-SEP-2003 (10)

## 2.2 Boiling Point

**Value:** = 210 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** Test conducted at a pressure of 15 mmHg
**Source:** Budavari 1996.
**Reliability:** (4) not assignable
24-SEP-2003 (1)

## 2.3 Density

**Value:** = .812 at 59 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** SIDS Dossier on 1-Octadecanol 1993b.
**Reliability:** (4) not assignable
30-SEP-2003 (12)

## 2.4 Vapour Pressure

**Value:** = .0000033 hPa at 25 degree C

**Method:** other (measured)
**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** Daubert and Danner 1989.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (2)

**Value:** = 1.33 hPa at 150.3 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** SIDS Dossier on 1-Octadecanol 1993b.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (12)

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** = 7.19

**Method:** other (measured)
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** A reverse-phase high pressure liquid chromatography/mass spectrometery method was used to estimate Kow in complex chemical mixtures.
**Source:** Burkhard et al. 1985.
**Reliability:** (2) valid with restrictions

## 2.6.1 Solubility in different media

**Solubility in:** Water
**Value:** = .0011 mg/l at 25 degree C

**Method:** other: measured
**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** Reported as insoluble in Budavari 1996.
**Source:** SIDS Dossier on 1-Octadecanol 1993b; Budavari 1996.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (1) (12)

## 2.7 Flash Point

**Value:** = 170 degree C

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** SIDS Dossier on 1-Octadecanol 1993b.
**Reliability:** (2) valid with restrictions
19-AUG-2003 (12)

## 2.9 Flammability

**Result:** other: moderate fire hazard

**Test substance:** other TS: Octadecanol (112-92-5)

**Source:** SIDS Dossier on 1-Octadecanol 1993b.
**Reliability:** (2) valid with restrictions
01-OCT-2003 (12)

## 3.5 Biodegradation

**Type:** aerobic
**Inoculum:** other: effluent from a domestic sewage treatment plant
**Concentration:** 2 mg/l related to Test substance
5 mg/l related to Test substance
**Contact time:** 29 day(s)
**Degradation:** = 69 - 38 % after 29 day(s)
**Result:** inherently biodegradable

**Method:** other: EEC Directive 92/69/EEC, C.4-E
**Year:** 1992
**GLP:** no data
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** This test method corresponds to OECD 301D.
**Remark:** Due to the low water solubility of the test substance, a homogenous distribution was achieved by ultrasound dispersion and stabilization by an inert emulsifier. The dispersing agent was nonylphenol ethoxylate additionally propoxylated with 5 propyleneoxide units (NP 9,5 EO 5PO). The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) oxygen depletion in the inoculum blank did not exceed 1.5 mg/l after 30 days, and (4) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.
**Result:** 7 days = 30 - 17%
14 days = 52 - 21%
21 days = 59 - 34%
28 days = 69 - 38%
Two concentrations of test material were tested: 2 mg/l and 5 mg/l. In the results section, the first values cited are for the 2 mg/l concentration and the second are for the 5 mg/l concentration.
The final result was greater than the 60% BOD/ThOD threshold but it did not reach this level within the 14 day window which is the criterion for classification of "ready biodegradability." At a test concentration of 5 mg/L the BOD/ThOD reached only 38% at 28 days. The reference substance, Sodium benzoate degraded by 88% after 29 days.
**Source:** Henkel KGaA 1992f.
**Test condition:** Inoculum concentration: 1 ml/l
Test volume: not reported
Temperature: 20 C
pH: not reported
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
29-OCT-2003 (7)

**Type:** aerobic
**Inoculum:** activated sludge
**Concentration:** 100 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 67 % after 28 day(s)
**Result:** inherently biodegradable

**Method:** other: ISO 10708 (BODIS)

**Year:** 1992
**GLP:** no data
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** The test method used is based on OECD test method 301D and the RDA-Blok-Test. It is especially suitable for poorly water-soluble compounds. The test medium is inoculated and the test chemical added. The test vessels are then closed and shaken continuously. Weekly measurements of the BOD from the aqueous phase are taken.
**Remark:** The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) the residual concentration of oxygen in the test bottle did not fall below 0.5 mg/l.
It could not be determined whether O2 depletion in the blank surpassed 1.5 mg/l after 28 days as no data was provided on Day 0 O2 concentrations.
**Result:** 7 days = 25%
14 days = 52%
21 days = 66%
28 days = 67%
The substance degraded <60% in the 14 day window. It took 20 days to degrade 60%. The reference substance, Sodium acetate, degraded by 86% after 28 days.
**Source:** Henkel KGaA 1992g.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
29-OCT-2003 (8)

**Type:** aerobic
**Inoculum:** other: no information on inoculum
**Concentration:** 20 mg/l related to Test substance
**Contact time:** 31 day(s)
**Degradation:** = 67 % after 31 day(s)
**Result:** inherently biodegradable

**Method:** other: US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test
**Year:** 1994
**GLP:** no data
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** This test followed the method set out in US EPA OPPTS 835.3100 Aerobic Aquatic Biodegradation Test (which corresponds to OECD 301B Modified Sturm Test) with one exception: after the samples were added, dichloromethane (30ml) was used to dissolve the non water-soluble alcohols. When the alcohol was dissolved the solvent was evaporated leaving an alcohol film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
**Remark:** There is no information given on the validity criteria.
**Result:** 4 days = 30%
10 days = 52%
17 days = 65%
24 days = 67%
31 days = 67%
The test substance attained <60% degradation during the 10

day window. Sodium benzoate was used as a positive control and reached a mineralization extent of 62.2%.
**Source:** Vista 1994.
**Test substance:** The substance corresponds to CAS# 112-92-5. Tradename is ALFOL 18.
**Reliability:** (2) valid with restrictions
Not key study: Other studies with higher reliability score and higher degradation rates are available.
31-OCT-2003 (15)

**Type:** aerobic
**Inoculum:** activated sludge, domestic
**Concentration:** 20 mg/l related to COD (Chemical Oxygen Demand)
**Contact time:** 28 day(s)
**Degradation:** = 43 % after 28 day(s)
**Result:** inherently biodegradable

**Method:** OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
**Year:** 1997
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** The test material was exposed to activated sewage sludge micro-organisms at a concentration of 20 mg C/l with culture medium in sealed culture vessels in the dark at 21 C for 28 days. The degradation of the test material was assessed by the determination of carbon dioxide produced. Control solutions with inoculum and the standard material, sodium benzoate were used for validation purposes.
**Remark:** The following validity criteria were met: (1) the parallel assays did not differ by more than 20%, (2) the reference compound reached the pass level within 14 days, (3) total CO2 evolution in the inoculum blank did not exceed 40 mg/l at the end of the test and (4) IC content of the test substance suspension in mineral medium at the start of the test was less than 5% of the total carbon.
**Result:** 8 days = 10%
14 days = 35%
20 days = 39%
28 days = 43%
The test material attained 43% degradation after 28 days and therefore cannot be regarded as readily biodegradable. The reference substance Sodium benzoate, attained 105% degradation after 28 days.
**Source:** Mead 1997d.
**Test substance:** This substance corresponds to CAS# 112-92-5. Tradename is Kalcol 8098.
**Reliability:** (1) valid without restriction
Not key study: Other studies (same reliability score) but with higher degradation rate are available.
10-SEP-2003 (11)

## 3.7 Bioaccumulation

**BCF:** = 100000

**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** The modeled estimate reported in the 1993 Dossier is considerably higher than the modeled estimate using the EPISuite model in 2000.
**Source:** SIDS Dossier 1993b.
**Reliability:** (2) valid with restrictions
25-SEP-2003 (12)

# AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

**Type:** semistatic
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**NOEC:** >= .4
**LC50:** > .4
**Limit Test:** yes

**Method:** OECD Guide-line 203 "Fish, Acute Toxicity Test"
**Year:** 1996
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** The solubility of octadecanol is estimated at about 0.001 mg/L, therefore the LC50 was not achieved at the solubility limit.
**Result:** RESULTS: EXPOSED
LC50 >0.40
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Wetton 1996d.
**Test condition:** TEST ORGANISMS
Strain: Oncorhynchus mykiss
Supplier: Donnington Fish Farm, Upper Swell, Gloucestershire, UK
Weight: 1.20 g
Feeding: commercial trout pellets
Pretreatment: Fish acclimatised to test conditions for 1 week prior to test
Feeding during test: None
Control group: 1 control group and 1 solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Tetrahydrofuran
Concentration of vehicle, solvent: 100 uL/L
STABILITY OF TEST CHEMICAL SOLUTIONS
Not reported
DILUTION WATER
Source: Dechlorinated laboratory tap water
Aeration: Test vessels aerated via narrow bore glass tubes
Alkalinity: 80 mg/l
Hardness: 136 mg/l CaCO3
Conductance: 382 MICSM
TEST SYSTEM
Concentrations: 0.4 mg/l
Renewal of test solution: Daily
Exposure vessel type: 20 l glass vessels
Number of replicates: 2
Fish per replicate: 10
Test temperature: 13-14 C
Dissolved oxygen: 9.2 - 10.1 mgO2/l
pH mean: 7.5 - 7.9
TEST PARAMETER: Mortality

SAMPLING: Mortalities and adverse reactions were recorded at

3, 6, 24, 48, 72 and 96 hours
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported

**Test substance:** Corresponds to CAS# 112-92-5. Tradename is Kalcol 8098.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
12-MAR-2004 (16)

**Type:** semistatic
**Species:** Brachydanio rerio (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**LC0:** = 10000
**LC50:** > 10000
**Limit Test:** no

**Method:** other: ISO 7346/II
**Year:** 1993
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Result:** RESULTS: EXPOSED
LC50 = >10000 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: none

Nature of adverse effects: mortality or sublethal effects
No mortality or sublethal effects were seen
Exposures were well in excess of water solubility limit.
**Source:** Stelter 1993.
**Test condition:** TEST ORGANISMS
Strain: Brachydanio rerio
Supplier: Westaquarium
Wild caught: no
Age/size/weight/loading: not reported
Feeding: Altromin N 1324
Pretreatment: none
Feeding during test: none
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into test vessels followed by 10 sec treatment with blender to disperse poorly soluble test substance.
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
REFERENCE SUBSTANCE: none
TEST SYSTEM
Concentrations: 0, 1000, 3000, 10000 mg/l
Renewal of test solution: daily
Exposure vessel type: 5 L aquarium

Number of replicates: 1
Fish per replicate: 10
Test temperature: 21.4 - 23.8C
Dissolved oxygen: 65-100% saturation
pH mean: 6.6-7.5
Adjustment of pH: not reported
Photoperiod: not reported

DURATION OF THE TEST: 96 h
TEST PARAMETER: mortality

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) but tested closer to the limit of water solubility are available

12-MAR-2004 (13)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** = 1000
**EC50:** = 1700
**EC100:** = 3000
**Limit Test:** no

**Method:** other: German Industry Standard DIN 38412, Part 11
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** METHOD FOLLOWED: German standard methods for the examination of water, waste water and sludge; bioassays (group L); determination of the effect of substances in water on microcrustaceans (Daphnia Shorttime Test)(L11). DIN 38412, Part 11.
This method corresponds to the OECD Guideline 202, part 1.
DEVIATIONS FROM GUIDELINE: not reported
STATISTICAL METHODS: not reported
METHOD OF CALCULATION: EC50 was calculated according to Stephan (square root of EC0 * EC100)

**Remark:** The solubility of C18 alcohol (Octadecanol) is about 0.001 mg/l, therefore the LC50 was not achieved at the solubility limit.

**Result:** RESULTS: EXPOSED
Nominal/measured concentrations: nominal
Effect data (Immobilisation): up to loadings of 1000 mg/l no immobilisation, at 3000 mg/l and 10000 mg/l 100% immobilisation
Effect concentration vs. test substance solubility: nominal loadings were well in excess of water solubility
RESULTS CONTROL: <10% mortality

**Source:** Guhl 1992e.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: own breed
Breeding method: not reported
Age: not reported
Feeding: green algae (Chlorella kessleri)
Pretreatment: not reported
Feeding during test: No
Control group: yes
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Dispersion: none
Vehicle, solvent: none
Other procedures: test substance was directly weighed into the test vessels
STABILITY OF THE TEST CHEMICAL SOLUTIONS: Dissolved Oxygen

Concentration (DOC) was measured for test substance concentrations of 1000 and 10000 mg/l and varied during the test between 0.3 and 0.5 mg/l (1000 mg/l) and 0.5-0.8 mg/l (10000 mg/l).
REFERENCE SUBSTANCE: not reported
DILUTION WATER:
Source: synthetic water according to DIN 38412, Part 11
TEST SYSTEM
Concentrations: 0, 10, 30, 100, 300 and 1000 mg/L
Renewal of test solution: No
Exposure vessel type: not reported
Number of replicates: not reported
Invertebrate per replicate: not reported
Test temperature: 20-21 C
Dissolved oxygen: 90-100% saturation
pH mean: 7.9-8.1
Adjustment of pH: not reported
DURATION OF THE TEST: 48 hours
TEST PARAMETER: Immbolization

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
12-MAR-2004 (3)

## 4.3 Toxicity to Aquatic Plants e.g. Algae

**Species:** Scenedesmus subspicatus (Algae)
**Endpoint:** biomass
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no
**EC10:** = 26
**EC50:** = 250
**Limit Test:** no

**Method:** other: DIN 38412, Part 9
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** Test method conforms with OECD-Guideline 201.
**Result:** RESULTS: EXPOSED
EC0 = < 10 mg/l (due to variability in cell density, the EC0 could not be reliably determined)
EC10 = 26 mg/l
EC50 = 250 mg/l
Based on nominal concentrations
The water solubility of Octadecanol is about 0.001 mg/l, therefore the EC50 is well above the solubility limit.
**Source:** Guhl 1992b.
**Test condition:** TEST ORGANISMS
Strain: Scenedesmus subspicatus
Supplier: Institute for plant physiology, University Gottingen
Pretreatment: not reported
Controls: 3 replicates
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: not reported
Concentration of vehicle, solvent: not reported
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported

DILUTION WATER
Source: not reported
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 10, 30, 100 and 300 mg/l (Unfiltered)
0.1, 0.3, 1.0, 3.0, 10.0 mg/l (Filtrate)
Exposure vessel type: 300 ml Erlenmeyer flasks
Number of replicates: 3
Initial cell concentration: 10000 cells/ml
Test temperature: 22-23.5 C
Dissolved oxygen: Not reported
pH mean: Not reported
Adjustment of pH: Not reported
Intensity of irradiation: 2000 Lux
Photoperiod: Constant illumination
TEST PARAMETER: biomass
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
12-MAR-2004 (5)

## 4.4 Toxicity to Microorganisms e.g. Bacteria

**Species:** Pseudomonas putida (Bacteria)
**Exposure period:** 30 minute(s)
**Unit:** mg/l **Analytical monitoring:** no data
**EC0:** > 10000

**Method:** other: OECD Oxygen Consumption Test
**Year:** 1994
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Remark:** German standard methods for the examination of water, waster water and sludge; bioassays (group L); determination of the inhibitory effect of waste water on the oxygen consumption of Pseudomonas putida (L 27); DIN 38412 part 27.
The oxygen consumption rate of a bacterial suspension fed glucose as nutrient base is measured after a contact time of 30 minutes. The oxygen consumption rate of the same bacterial suspension in the presence of various concentrations of a test substance under otherwise identical conditions is also measured.
This information is additional to that reported in the 1993 SIDS dossier prepared by the Environment Protection Agency of Denmark.
The water solubility of the compound is approximately 0.001 mg/l, therefore the EC50 was not achieved at the solubility limit.
**Source:** Henkel KGaA, 1994c
**Test substance:** This substance corresponds to CAS #112-92-5. Tradename is Lorol C18-98.
**Reliability:** (1) valid without restriction
Best study although not a SIDS endpoint.
30-OCT-2003 (9)

**Species:** other bacteria: Streptococcus mutans
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**MIC :** > 100

**Method:** other
**Year:** 1987
**GLP:** no data
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** Two fold dilutions of Fatty alcohols were prepared by diluting the original methanolic solutions (2 mg/ml) with the same solvent. The dilutions (0.1 ml each) were added to brain heart infusion broth containing precultures S. mutans cells (ca. 10E6 cells/ml). The mixtures were cultured for 48 h at 37 C. MICs were determined by visually judging the bacterial growth in the series of test tubes.
The experiments were carried out in triplicate.
**Remark:** MIC = Minimal Inhibitory Concentration
The SPARC estimated water solubility of Octadecanol is 0.00066 mg/l, therefore MIC concentration appears to be above the saturation limit.
**Source:** Hattori et al. 1987.
**Reliability:** (3) invalid
Not key study: Other studies with higher reliability score are available
25-SEP-2003 (6)

## 4.5 Chronic Toxicity to Aquatic Organisms

## 4.5.2 Chronic Toxicity to Aquatic Invertebrates

**Species:** Daphnia magna (Crustacea)
**Endpoint:** other: reproduction rate and mortality
**Exposure period:** 21 day(s)
**Unit:** mg/l **Analytical monitoring:** yes
**NOEC:** = .98
**LOEC:** = 2.94

**Method:** other: comparable to OECD Guide-line 202, part 2 "Daphnia sp., Reproduction test"
**Year:** 1992
**GLP:** yes
**Test substance:** other TS: Octadecanol (112-92-5)

**Method:** Chronic toxicity testing in Daphnia magna according to UBA toxicity testing protocol 'Prolonged toxicity test with Daphnia Magna', 01.02.1984; determination of the NOEC for reproduction rate, mortality and the moment of the first appearance of descendants.
**Remark:** Data refer to both mortality of parents and number of offspring/parent. The test substance was added directly, without the use of solvents. Note that the NOEC is approximately 100 times the solubility of octadecanol in water. Test conducted in 1992.
**Result:** RESULTS:

| Concentration (mg/L) | 0 | 1 | 3 | 10 | 30 | 100 |
|---|---|---|---|---|---|---|
| First day of offspring | 9-12 | 9-12 | 9-12 | 9-12 | 9-12 | 9-12 |
| Survival rate of adults (%) | 90 | 90 | 70 | 70 | 60 | 55 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Average number of young animal per adult | 106 | 101 | 81 | 56 | 56 | 45 |
| Standard deviation | 3.5 | 21.5 | 17.6 | 20.7 | 8.6 | 12.1 |
| Significant (p<0.05) | -- | no | yes | yes | yes | yes |

NOEC = 0.98 mg/L
LOEC = 2.94 mg/L

CONTROL SUBSTANCE:
No use of control substance reported.

**Source:** Guhl 1992.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: Own breeding, strain is identical with that of BGA
Age: not reported
Feeding: 1 ml algae (1-3 * 10E6 cells/ml) and 1 ml activated sludge
Feeding during test: Monday/Wednesday/Friday
Control group: 1 group (4 replicates)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: none (test substance was weighed directly into test vessels)
Concentration of vehicle/solvent: not applicable
DILUTION WATER
Source: Aerated tap water
Aeration: not reported
Alkalinity: not reported
Hardness: not reported
Conductance: not reported
TEST SYSTEM
Concentrations: 1, 3, 10, 30 and 100 mg/l
Renewal of test solution: Monday/Wednesday/Friday
Exposure vessel type: 500 ml Erlenmeyer flasks
Number of replicates: 4
Animals per replicate: 5
Test temperature: 19-23 C
Dissolved oxygen: not reported
pH mean: 8.3-8.5
Adjustment of pH: not reported
Intensity of irradiation: Radium 60W
Photoperiod: 16 hours light, 8 hours dark
TEST PARAMETER: reproduction rate and mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: 0, 48 and 120 hours. Mean measured (DOC) concentrations in the 10 mg/l group were 0.7, 1.15 and 1.95 mg/l at 0, 48 and 120 hours, respectively. Similar measured concentrations were obtained in the 30 and 100 mg/l groups.

**Reliability:** (2) valid with restrictions
Best study although not a SIDS endpoint.

30-OCT-2003 (4)

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

| | | |
|---|---|---|
| **Test substance** | : | n-hexanol; n-heptanol; n-octanol; n-nonanol; n-decanol; n-octadecanol |
| **Test condition** | : | These studies were carried out to determine the extent to which various monohydric aliphatic alcohols, including C6-C18 alcohols included in this category, form glucuronic acid conjugates in the rabbit.<br><br>Groups of 3 Chinchilla rabbits, about 3 kg in weight, were administered various alcohols in water by gavage at a dose level of 25 m.moles/rabbit. The excretion of glucuronic acids was determined daily in the urine for a week prior to administration of the test compound to establish a base line. Following dosing the urine was collected for 24 hours and the glucuronides extracted.<br><br>The results were reported as the amount of extra glucuronic acid excreted as a % of dose. |
| **Result** | : | The extra glucuronide excreted as % of dose (average of 3 rabbits, 2 rabbits for *) was as follows:<br><br>n-hexanol 10.3%; n-heptanol 5.3%; n-octanol 9.5%; n-nonanol 4.1%; n-decanol* 3.5%; n-octadecanol* 7.6%. It was reported that absorpton of n-decanol and n-octadecanol was incomplete and irregular and the alcohol could be isolated in quantity from the faeces.<br><br>No further information on other biotransformation pathways of these alcohols was provided. |
| **Conclusion** | : | All the primary alcohols investigated form glucuronic acid conjugates which are excreted in the urine. However this was generally <10% of the dose. |
| **Reliability** | : | (2) valid with restrictions |
| **Source** | : | Kamil et al, 1953<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |

08.07.2005 (15)

## 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | rat |
| **Strain** | : | Wistar |
| **Sex** | : | male/female |
| **Number of animals** | : | 10 |
| **Vehicle** | : | other: 50% suspension in DMSO |
| **Value** | : | > 5000 mg/kg bw |
| **Method** | : | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year** | : | 1981 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Lorol/Lanette 18 |
| **Test condition** | : | TEST ORGANISMS: rat (Wistar)<br>- Source: Winkelmann, Hanover, Germany<br>- Weight at study initiation: average body weight males 177g, females |

141g.
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: gavage
- Doses: 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: 10 ml/kg as a 50% suspension in DMSO.
- Post dose observation period: 14 days.

EXAMINATIONS: Mortality and clinical signs were recorded. Body weights were taken before dosing and at 24 hours, 1 and 2 weeks after dosing. All rats were subject to gross necropsy at the end of the observation period.

**Result** : MORTALITY: All animals survived the observation period.

CLINICAL SIGNS: Directly after application the animals showed moderate piloerection and slight sedation. These effects vanished completely within 24 hours. Group body weights increased over the observation period.

NECROPSY FINDINGS: Round deposits of test substance remained in the stomach. There were no other gross pathological observations.

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None.

**Conclusion** : The rat oral LD50 for Lorol (Lanette) 18 was >5000 mg/kg. Signs of intoxication were confined to transient mild sedation and moderate piloerection.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Henkel KGaA 1981g
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (12)

**Type** : LD50
**Species** : rat
**Strain** : other: Holzman
**Sex** : male/female
**Number of animals** : 5
**Vehicle** : other: 20% w/v corn oil suspension
**Value** : > 7960 mg/kg bw
**Method** : other: contract laboratory protocol.
**Year** : 1965
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Alfol 12

**Test condition** : TEST ORGANISMS: Rat (Holtzman)
- Weight at study initiation: 205-254 g
- Group size: 5M+5F no indication as to whether the animals were fasted.
- Controls: No

ADMINISTRATION: GAvage
- Doses: 2.0 and 7.96 g/kg

- Doses per time period: single
- Volume administered or concentration: 20% suspension in corn oil.
- Post dose observation period: 14 days

EXAMINATIONS: Mortality and clinical signs frequently on day of dosing, thereafter daily. Bodyweights were recorded at study initiation and at the end of the observation period. Gross necrospy was carried out on all animals at the end of the observation period.

**Result** : MORTALITY: There were no mortalities at any dose level.

CLINICAL SIGNS: No signs of toxicity or pharmacological effects were observed at the low test level. Diarrhoea was observed in most animals at the higher dose level at 24 hours. All animals appeared normal within 48 hours. All animals gained weight within the normal limits.

NECROPSY FINDINGS: Gross necropsy of the animals sacrificed at termination did not reveal any remarkable findings.

POTENTIAL TARGET ORGANS: None identified.
SEX-SPECIFIC DIFFERENCES: None reported.

**Conclusion** : The rat oral LD50 of Alfol 18 is >7960 mg/kg. Other than diarrhoea at the top dose level there were no clinical or gross pathological signs toxicity.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Scientific Associates, Inc. 1965f
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (21)

**Type** : LD50
**Species** : rat
**Strain** : other: Sprague-Dawley CD
**Sex** : male/female
**Number of animals** : 10
**Vehicle** : other: arachis oil
**Value** : > 2000 mg/kg bw
**Method** : OECD Guide-line 401 "Acute Oral Toxicity"
**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Kalcol 8098

**Test condition** : TEST ORGANISMS: Rat (Sprague-Dawley)
- Source: Charles River, Margate, Kent, UK
- Age: 5-8 weeks
- Weight at study initiation: males 135-145g, females 127 -137g
- Group size: 5M+5F fasted
- Controls: no

ADMINISTRATION: Gavage
- Doses: Single dose level of 2000 mg/kg based on a range finding test.
- Doses per time period: single dose
- Volume administered or concentration: 200 ml/kg at a concentration of 10mg/ml in arachis oil. Preparation of the solution was aided by warming in a water bath.

- Post dose observation period: 14 days

EXAMINATIONS: The rats were observed for clinical signs of toxicity and mortality at 30 minutes, 1, 2 and 4 hours after dosing and thereafter daily throughout the observation period. Body weights were recorded prior to dosing on day 0 and then at 7 and 14 days. All animals were subject to both pathological examination at the end of the observation period.

**Result** : MORTALITY: There were no deaths.

CLINICAL SIGNS: No clinical signs of systemic toxicity. All animals showed the expected body weight gain over the observation period.

NECROPSY FINDINGS: Unremarkable

POTENTIAL TARGET ORGANS: None identified.

SEX-SPECIFIC DIFFERENCES: None observed.

**Conclusion** : The rat oral LD50 fro Kalcol 8098 is >2000 mg/kg. There were no signs of toxicity.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Hempstock 1996b
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

11.08.2005 (10)

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

**Remark** : Not required OECD or HPV endpoint.

**Source** : The Weinberg Group Inc. Washington D.C
Shell Chemicals Ltd. London
Hayes Consultancy Service Bromley, Kent

07.03.2000

### 5.2.1 SKIN IRRITATION

**Species** : other: New Zealand White rabbit
**Concentration** :
**Exposure** : Semiocclusive
**Exposure time** : 4 hour(s)
**Number of animals** : 3
**PDII** : 0
**Result** : not irritating
**EC classification** : not irritating
**Method** : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

| | | |
|---|---|---|
| **Test substance** | : | Tradename Kalcol 8098 |
| **Test condition** | : | TEST ANIMALS: Rabbit<br>- Strain: New Zealand White<br>- Sex: Female<br>- Source: David Percival Ltd, Cheshire, UK<br>- Age: 12-16 weeks<br>- Weight at study initiation: 2.56 - 2.73 kg<br>- Number of animals: 3<br><br>ADMINISTRATION/EXPOSURE<br>- Preparation of test substance: The test material was a white solid, the test site was moistened with 0.5 ml distlled water prior to application of 0.5 g of the solid.<br>- Area of exposure: 2.5 x 2.5 cm<br>- Occlusion: semi-occlusive<br>- Vehicle: None<br>- Total volume applied: 0.5 g<br>- Exposure period: 4 hours<br>- Postexposure period: 72 hours<br>- Controls: None reported<br><br>EXAMINATIONS<br>- Scoring system: Draize<br>- Examination time points: 24, 48 and 72 hours post application |
| **Result** | : | The test material produced a primary irritation index of 0.0. No evidence of skin irritation was noted during the study, all scores were 0. |
| **Conclusion** | : | Following a 4 hour semi-occlusive exposure to rabbits skin Kalcol 8098 was non-irritating to rabbit skin. |
| **Reliability** | : | (1) valid without restriction<br>Guideline study |
| **Source** | : | Sanders 1996c<br>Hayes Consultancy Service Bromley, Kent |
| **Flag** | : | Critical study for SIDS endpoint |

11.08.2005 (18)

### 5.2.2 EYE IRRITATION

| | | |
|---|---|---|
| **Species** | : | other: New Zealand White rabbit |
| **Concentration** | : | undiluted |
| **Dose** | : | .1 ml |
| **Exposure Time** | : | |
| **Comment** | : | not rinsed |
| **Number of animals** | : | 3 |
| **Result** | : | not irritating |
| **EC classification** | : | not irritating |
| **Method** | : | OECD Guide-line 405 "Acute Eye Irritation/Corrosion" |
| **Year** | : | 1987 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Kalcol 8098 |
| **Test condition** | : | TEST ANIMALS: Rabbit<br>- Strain: New Zealand White |

- Sex: 1 male, 2 females
- Source: David Percival Ltd, Cheshire, UK
- Age: 12-16 weeks
- Weight at study initiation: 2.90-3.23 kg
- Number of animals: 3
- Controls: Untreated eye used as control

ADMINISTRATION/EXPOSURE
- Preparation of test substance: the substance was a solid and was applied using an adapted syringe.
- Amount of substance instilled: 0.1 ml (ca 82 mg)
- Vehicle: None
- Postexposure period: 72 hours

EXAMINATIONS
- Scoring system: Draize and modified Kay and Callandra.
- Observation period: 72 hours
- Tool used to assess score: Standard ophthalmoscope.

**Result** : AVERAGE SCORE (24+48+72 hour)
- Cornea: 0, 0, 0.3 (group mean score 0.1)
- Iris: 0, 0, 0.3 (group mean score 0.1)
- Conjunctivae (Redness): 0.3, 0, 1 (group mean score 0.43)
- Conjunctivae (Chemosis): 0, 0, 0.3 (group mean score 0.1)
- Overall irritation score: maximum group mean score 10.0 at 1 hour post instillation. Classified as a mild irritant.

DESCRIPTION OF LESIONS: The application of the test material produced diffuse corneal opacity restricted to one treated eye at 24 hours. Iridial inflammation was noted in 2 eyes at 1 hour and one at 24 hours. Minimal to moderate conjunctival irritation was reported at 1 hour with minimal conjunctivitis in 2 eyes at 24 hours.

REVERSIBILITY: All eyes scored 0 at 48 and 72 hours post instillation.

OTHER EFFECTS: Residual test material noted around all eyes at the 1 hour observation period.

**Conclusion** : Kalcol 8098 is not an eye irritant according to EU or GHS criteria.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Sanders 1996h
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

04.01.2006 (19)

## 5.3 SENSITIZATION

**Type** : Guinea pig maximization test
**Species** : other: albino Dunkin Hartley guinea pig
**Concentration** : Induction 1 % intracutaneous
Induction 50 % occlusive epicutaneous
Challenge occlusive epicutaneous
**Number of animals** : 10
**Vehicle** : other: arachis oil
**Result** : not sensitizing
**Classification** : not sensitizing
**Method** : OECD Guide-line 406 "Skin Sensitization"

**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Kalcol 8098

**Test condition** : TEST ANIMALS: Guinea pigs
- Strain: Dunkin Hartley
- Sex: male
- Source: David Hall, Staffs, UK
- Age: 8-12 weeks
- Weight at study initiation: 305 -419 g
- Number of animals: 10
- Controls: 5

ADMINISTRATION/EXPOSURE
- Study type: M&K maximisation procedure (adjuvant method)
- Preparation of test substance for induction: in arachis oil
- Induction schedule: Day 1 intradermal induction, day 7 topical induction (48 hours occlusive).
- Concentrations used for induction: intradermal 1% in arachis oil, topical 50% in arachis oil.
- Concentration in Freuds Complete Adjuvant (FCA): 1%
- Challenge schedule: Day 21 topical challenge (24 hours occlusive)
- Concentrations used for challenge: 25 and 50% in arachis oil.
- Rechallenge: No
- Positive control: Evidence of reaction of the strain of guinea pigs to known skin sensitisers over an appropriate period was provided.

EXAMINATIONS
- Grading system: Draize 0-4 scale for erythema and oedema.
- Pilot study: Topical (24 and 48 hour occlusive) applications were tested at 5, 10, 25 and 50%. Intradermal injection was attempted at 1 and 5% but the 5% solution was impossible to inject.

**Result** : RESULTS OF PILOT STUDY: Minimal erythema at 24 and 48 hours after 48 hour topical exposure, no irritation at these time periods after a 24 hour topical application. Well defined erythema (grade 2) at 24, 48 and 72 hours post injection reducing to slight erythema (grade 1) at 7 days.

RESULTS OF TEST
- Sensitization reaction: No positive responses with 25% or 50% challenge concentrations in test or control groups at 24 or 48 hours. 0/10 treated and 0/5 controls responded to challenge.
- Clinical signs: Body weights and weight gain over the observation period were comparable in test and control groups. Well-defined erythema was noted at the intradermal induction sites of all test group animals at 24 and 48hours. Very slight to well-defined erythema was noted at the intradermal sites of the control group at 24 and very slight erythema at 3 sites at 48 hours.
Very slight to well-defined erythema was noted at the induction sites of six test group animals at the 1 hour mark. No skin reactions were noted at the induction sites of any test group animals at the 24 hour mark.
- Rechallenge: Not carried out.

**Conclusion** : Kalcol 8098 is not a skin sensitiser when tested using the Magnusson and Kligman guinea pig maximization procedure.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Driscoll 1996b
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
07.12.2005 (6)

## 5.4 REPEATED DOSE TOXICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | male/female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 28 days |
| **Frequency of treatment** | : | daily, 5 days/week |
| **Post obs. period** | : | 28 days |
| **Doses** | : | 0, 100, 500, 1000 mg/kg in olive oil |
| **Control group** | : | yes, concurrent vehicle |
| **NOAEL** | : | = 1000 mg/kg bw |
| **Method** | : | OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study" |
| **Year** | : | 1986 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Tradename Lanette 18 |

**Test condition** :

TEST ORGANISMS
- Supplier: Charles River Wiga GmbH, Sulzburg
- Age/Weight at study initiation: M64-97 g; F 62-99g
- Number of animals: 10M+10F per dose level plus 5M+5F per dose level for reversibility.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 27-28 days exposure (5 days/week)
- Type of exposure: oral gavage
- Post exposure period: 28 days
- Vehicle: Olive oil
- Concentration in vehicle: 0, 2, 10 or 20%
- Total volume applied: 5 ml/kg
- Doses: 0, 100, 500 and 1000 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: 5M+5F per dose level for reversibility.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Ad lib
- Ophthalmoscopic examination: At end of study
- Haematology: After 21/22 daily doses: Haematocrit, MCV, Hb, RBC, WBC, Thrombocytes, differential white count.
- Biochemistry: After 21/22 daily doses: Serum Urea, creatinine, Na, K, calcium, alkaline phosphatase, ALAT, ASAT, GT, bilirubin, chloride, Albumin, total protein, chloesterol.
- Urinalysis: Not done

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND

MICROSCOPIC):
- Macroscopic: Yes
- Organs weights: thyroid, adrenals, thymus, kidney, spleen, heart, brain, testes, liver.
- Microscopic: All organs from the control and top dose animals were examined plus the animals from the reversibility study.

STATISTICAL METHODS: T-test, organ weights U-test.

**Result** **:** NOAEL: 1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
0, 100, 500 & 1000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: No mortalities.
- Clinical signs: Unremarkable.

- Body weight gain: Male bodyweight gain was reduced compared to controls, body weight gains were 95%, 91% and 82% of control values for low, mid and high dose levels respectively at the end of the study. This was attributed to a high mean control bodyweight in males and marked inhibition of bodyweight gain in one male in each of the high and mid dose levels.

- Food/water consumption: Water consumption was comparable in control and treated groups. Food consumption was slightly reduced in males (95% confidence).

- Ophthalmoscopic examination: No treatment related ocular lesions.

- Clinical chemistry: There were some statistically significant changes (p=0.05) in clinical chemical parameters in the top dose group. In males ASAT was increased (control mean 33 U/l; top dose 45.1); Na was also increased (control mean 143.1 mmol/l; top dose 144.4). Serum chloride was reduced (control mean 99.7 mmol/l; top dose 97.9). In females there was an increase in Na (control mean 142 mmol/l; top dose 143) and in phosphorous (control mean 1.99 mmol/l; top dose 21.9. These changes are not clearly dose related and apart from the slight increase in serum sodium do not appear in both sexes. There are no histopathological changes related to these changes which were considered chance observations and not indicative of a trend.

- Haematology: Treated and control groups were comparable. A slight increase (95% confidence *) in neutrophils with rod-like bodies (mid dose males), a marginal decrease in thrombocytes (top dose males) and eosinophils (top dose females) were not considered of biological significance.

Thrombocytes:

| | Control | low | mid | high |
|---|---|---|---|---|
| male | 633.9 | 619.9 | 583.9 | 511.9* |

Eosinophils:

| | | | | |
|---|---|---|---|---|
| female | 1.3 | 0.8 | 0.9 | 0.3** |

- Urinalysis: Not done

- Organ weights: Sporadic changes in absolute or relative organ weights relative weights were not dose and/or sex related. There was no

corresponding histopathological change. Relative heart weights were increased* in top dose males, Relative and absolute kidney weights were decreased* in mid-dose females, while other absolute organ weights were changed as follows:

Absolute mean spleen weight:

| | Control | low | mid | high |
|---|---|---|---|---|
| male | 0.706 | 0.651 | 0.585* | 0,593* |

Absolute mean thyroid weight:

| | Control | low | mid | high |
|---|---|---|---|---|
| male | 0.024 | 0.018** | 0.02 | 0.018** |

Absolute mean spleen weight:

| | Control | low | mid | high |
|---|---|---|---|---|
| male | 0.706 | 0.651 | 0.585* | 0.593* |

Relative mean heart weight:

| | Control | low | mid | high |
|---|---|---|---|---|
| male | 0.281 | 0.288 | 0.302 | 0.314* |

- Pathology: There were no treatment related findings. Pathological changes observed were related to misdosing, respiratory infection or viral infection.

STATISTICAL RESULTS: T-test and U-test for organ weights.

**Conclusion** : The NOAEL for this study is considered to be >1000 mg/kg/day based on a lack of toxicologically significant effects. Statistically significant changes in some clinical chemical and haematological parameters and organ weights changes were not accompanied by histopathological changes and were either not dose related or appeared in only one sex. These effects are not considered of toxicological significance.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Henkel KGaA 1986a; Henkel 1999 (2-page English summary)
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
04.01.2006 (13) (14)

**Species** : rat
**Sex** : male/female
**Strain** : Wistar
**Route of admin.** : oral feed
**Exposure period** : males 45 days; females ca 54 days
**Frequency of treatment** : continuous in diet
**Post obs. period** : none
**Doses** : 0, 1500, 7500 or 30,000 ppm (ca 0, 100, 500, 2000 mg/kg/bw/day)
**Control group** : yes
**NOAEL** : = 2000 mg/kg bw
**Method** : other: Draft OECD 422 combined repeated dose and reproductive/developmental toxicity screening test
**Year** : 1991
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS
- Age: 7 weeks

- Number of animals: 12M+12F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: males: 45 days; females approx. 54 days
- Type of exposure: Dietary
- Post exposure period: None
- Vehicle: Diet. Diet preparation involved first mixing the octadecanol with the barley component, the proportion of which varied for each dose level. The other components of the diet were then added.

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality: Daily
- Body weight: weekly
- Food consumption: weekly (except during mating)
- Water consumption: ad lib
- Haematology: Males only at day 37; haematocrit, Hb, total RBC & WBC and differential WBC.
- Biochemistry: Males only at day 37; Plasma protein, alkaline phosphatase, AAT, glucose, urea, creatinine,total & free cholesterol and triglyceride.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full necrospy on all animals.
- Organ weights: liver, kidneys, thymus (females) liver, kidney, thymus, testes, epididymes (males)
- Microscopic: Carried out on all control and top dose animals plus any obvious lesions observed at necrospy. Organs examined were liver, kidneys, adrenals, brain, heart, spleen, ovaries or testes and epididymes.

OTHER EXAMINATIONS: The results of foetal examinations and reproductive parameters are reported in the appropriate sections.

STATISTICAL METHODS: Using the SAS-stat program analysis of variance plus Dunnett's test if changes were significant.

**Result** **:** NOAEL 2000 mg/kg/day, LOEL: 100 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX
Males: 99.25, 500.25 and 2146.5 mg/kg/day (mean of values reported for 2 weeks prior to mating and 3 weeks after mating)
Females:120, 625 and 2435.5 mg/kg/day (mean of values reported 2 weeks prior to mating)

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: There were no mortalities.
- Clinical signs: None reported.

- Body weight gain: There were no significant changes in body weight or body weight gain in the 3 weeks prior to mating for both sexes. Or in males after mating.

- Food consumption/efficiency: Food consumption was significantly increased in top dose males ($p<0.001$) and in mid dose females ($p<0.05$) at week 3. There were no other differences in food consumption or food conversion efficiency.

- Clinical chemistry: (males only examined) There were significant (but non-dose related) differences in free cholesterol (increased) and triglycerides (decreased) at all dose levels. Total cholesterol levels were not significantly

increased. Plasma glucose was elevated with statistical significance in the low and mid-dose groups.

| Parameter (mM) | Control | 100 | 500 | 2000 |
|---|---|---|---|---|
| Free chol | 0.29 | 0.38** | 0.37** | 0.36* |
| Total chol | 1.30 | 1.56 | 1.56 | 1.40 |
| Triglycerides | 0.78 | 0.42** | 0.49* | 0.46** |
| Glucose | 6.8 | 7.8* | 7.9* | 7.6 |

* p<0.05 ** P<0.01

- Haematology: No statistically significant differences between treated and control groups (males only examined).
- Organ weights: There were no significant differences in absolute or relative organ weights in males or females.

- Gross pathology: Unremarkable no changes attributable to treatment.
- Histopathology: Unremarkable no changes attributable to treatment.

- Other: The method of diet preparation resulted in different dietary content between the different treatment groups and controls.

STATISTICAL RESULTS: Reported above.

**Conclusion** : The only systemic effects seen in this study were significant changes in plasma free cholesterol, triglycerides and glucose. These changes occurred at all dose levels but were not dose related. Although the reduction in plasma triglycerides levels may be indicative of mild effects in the liver, the differences in the composition of the test diets may have confounded these results. The NOAEL can be considered to be 2000 mg/kg/day with a NOEL of 100 mg/kg/day.

**Reliability** : (2) valid with restrictions
comparable to guideline study (draft guideline) with acceptable restrictions

**Source** : Hansen 1992b.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

03.01.2006 (9)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Bacterial reverse mutation assay
**System of testing** : Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, and TA 100
**Concentration** : 50 to 5000 ug/plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : OECD Guide-line 471
**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Kalcol 8098

**Test condition** : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 1535, TA 1537, TA 1538, TA 98, and TA 100
- Deficiences/Proficiences: Histidine deficient

- Metabolic activation system: Rat liver S9 Arocholor 1254 induced

ADMINISTRATION:
- Dosing: 50, 150, 500, 1500 and 5000 ug/plate.
- Number of replicates: Duplicate tests each performed in triplicate
- Application: Plate incorporation assay, vehicle ethanol.
- Positive and negative control groups and treatment: Vehicle control-ethanol. Postive controls without S9- N-ethyl-N'-nitrosoguanidine 3 ug/plate (TA100), 5ug/plate (TA1535), 9-aminoacridine 80 ug/plate (TA1537), 4-nitro-o-phenylene diamine 5ug/plate (TA 1538), 4-nitroquinoline-1-oxide 0.2 ug/plate (TA98). with S9 2-aminoanthracene (0.5, 1 or 2 ug/plate).
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: A dose related and statistically significant increase in reverse mutation rate in one or more bacterial strains at sub-toxic dose levels. For a negative result the numbers of induced revertants should be less than two fold compared to controls.

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate in any strain at dose levels up to 5000 ug/plate. Positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: >=500 ug/plate but this did not interfere with scoring of the plate, plates were counted manually at 5000 ug/plate.

CYTOTOXIC CONCENTRATION: There was no evidence of cytotoxicity up to 5000 ug/plate with or without S9.

STATISTICAL RESULTS: Dunnetts test was used and showed no statistically significant differences between test and control plates.

**Conclusion** : The C18 alcohol Kahlcol 8098 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 5000 ug/plate. This dose level was not cytotoxic.

**Reliability** : (1) valid without restriction
Guideline study

**Source** : Thompson 1996d
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

12.08.2005 (24)

**Type** : other: Bacterial reverse mutation assay (Ames Test)
**System of testing** : Strains TA 100, TA 1535, TA 1537, TA 1538, TA 98
**Concentration** : 4, 20, 100, 500, 2500 ug/plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: An in-house protocol based on OECD Guide-line 471
**Year** : 1982
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Lanette 18

**Test condition** : METHOD: Bacterial reverse mutation assay similar to OECD 471. Full experimental details were not provided but actual results were available. 2-

aminoanthracene was the only indicator of efficacy of the S9 mix however there was a clear increase in reverse mutation rate in bacteria treated with 2-AA in the presence of S9 compared to controls. The test was not repeated.

SYSTEM OF TESTING:
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538
- Deficiences/Proficiences: histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: 0, 4, 20, 100, 500, and 2500 ug/plate aqueous suspension using Tween 80.
- Number of replicates: Duplicates. One test only.
- Application: Plate incorporation. Vehicle aqueous suspension in Tween 80.
- Positive and negative control groups and treatment: Positive controls were 2-amino anthracene 5 ug/plate, sodium azide 1 ug/plate; 4-nitro-o-phenylene diamine 40 ug/plate.

CRITERIA FOR EVALUATING RESULTS: Not specifically reported assume as OECD 471.

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: There was no increase in reverse mutation rate in any of the test strains at any dose level, positive and negative controls gave appropriate responses.

PRECIPITATION CONCENTRATION: None reported

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: Slight cytotoxicity observed at 2500 ug/plate as evidenced by reduction in numbers of revertants in strains TA98 and 100.

**Conclusion** : The C18 alcohol Lanette 18 did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels up to 2500 ug/plate. Slight cytotoxicity was evident at 2500 ug/plate.

**Reliability** : (2) valid with restrictions
Comparable to guidleine study with acceptable restrictions

**Source** : Henkel KGaA 1981f.

Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

12.08.2005 (11)

**Type** : other: Bacterial reverse mutation assay (screening test)
**System of testing** : Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537
**Concentration** : 3 umol/plate (spot test)
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: Ames test
**Year** : 1980
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced. Activity tested using 2-aminoanthracene.

ADMINISTRATION:
- Dosing: 3 umol/plate
- Number of replicates: not reported
- Application: Spot test screening only
- Positive and negative control groups and treatment: 2-aminoanthracene and N-methyl-N'-nitrosoguanidine.

CRITERIA FOR EVALUATING RESULTS: Not reported.

**Result** : GENOTOXIC EFFECTS:
- With or without metabolic activation: Reported as not mutagenic but precipitation of the test material made the results difficult to evaluate.

PRECIPITATION CONCENTRATION: 3 umol/plate

CYTOTOXIC CONCENTRATION:
- With and without metabolic activation: No significant cytotoxicity at the concentration tested.

**Conclusion** : This test with octadecanol is a screening test and of limited value especially as precipitation made interpretation difficult. However the test was reported as negative.

**Reliability** : (3) valid with restrictions
Publication, results reported for a number of chemicals including octadecanol, limited data presented.

**Source** : Florin, 1980

Hayes Consultancy Service Bromley, Kent

12.08.2005 (7) (23)

**Type** : other: bacterial reverse mutation assay screening test
**System of testing** : Salmonella typhimurium strains TA98, TA100, TA1535, TA1537, and TA1538
**Concentration** : 50 ug/spot
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: Ames et al, 1975
**Year** : 1982
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538
- Deficiences/Proficiences: Histidine deficient.
- Metabolic activation system: Rat liver S9 Arochlor 1254 induced.

ADMINISTRATION:
- Dosing: Spot test at a single concentration of 50 ug.
- Number of replicates: Not replicated, screening test only.
- Application: Spot test assay, vehicle sterile double distilled water.

- Positive and negative control groups and treatment: Vehicle control and 2-aminoanthracene to demonstrate activity of the S9 metabolising fraction. No other positive controls.
- Incubation time: 48 hours at 37C.

CRITERIA FOR EVALUATING RESULTS: Increase in revertants over control levels with significant dose-related increase over controls.

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: No evidence of increased reverse mutation in any strain in this screening (spot) test. Appropriate responses were obtained with positive and negative controls.

PRECIPITATION CONCENTRATION: Not reported

CYTOTOXIC CONCENTRATION: By inference a non-cytotoxic concentration (50 ug/spot) was chosen for this screening test.

**Conclusion** : Stearyl aclohol (C18) was evaluated in a screening (spot) test using histidine deficient strains of Salmonella typhimurium. There was no evidence of mutagenic activity with or without metabolising fraction.

**Reliability** : (4) not assignable
Publication, results reported for a number of chemicals including octadecanol, acceptable for assessment.

**Source** : Blevins et al, 1982
Hayes Consultancy Service Bromley, Kent

12.08.2005 (3) (23)

**Type** : Bacterial reverse mutation assay
**System of testing** : Salmonella typhimurium strains TA1535, TA1537, TA 1538, TA98, TA100
**Concentration** : 0.63, 1.25, 2.5, 5, 10 and 20 ug/plate
**Cycotoxic conc.** :
**Metabolic activation** : with and without
**Result** : negative
**Method** : other: Ames test (Japanese Ministry of Labour protocol)
**Year** : 1982
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Octadecanol CAS RN 112-92-5 (Kalcohl 80, 718)

**Test condition** : SYSTEM OF TESTING
- Species/cell type: Salmonella typhimurium strains TA1535, TA1537, TA 1538, TA98, TA100
- Deficiences/Proficiences: Histidine deficient
- Metabolic activation system: rat liver cells, KC500 induced...

ADMINISTRATION:
- Dosing: 0.63, 1.25, 2.5, 5, 10 and 20 ug/plate
- Number of replicates: Single test performed in duplicate.
- Application: Vehicle DMSO
- Positive and negative control groups and treatment: Positive controls: N-ethyl-N'-nitro-N-nitrosoguanidine 10 ug/plate; 4-nitroquinoline 0.5 ug/plate; 2-nitrofluorene 5 ug/plate; 9-aminoacridine 50 ug/plate; 2-aminoanthracene 2 ug/plate. Not stated whether the controls were untreated or solvent controls.
- Incubation time: preincubation for 20 minutes, incubation of plats for 48 hours.

CRITERIA FOR EVALUATING RESULTS:

**Result** : GENOTOXIC EFFECTS:
- With and without metabolic activation: No increase in reverse mutation rate.

PRECIPITATION CONCENTRATION: None reported.

CYTOTOXIC CONCENTRATION: Test concentrations were determined by solubility in phosphate buffer at the preincubation stage. There was no significant reduction in background lawn.

**Conclusion** : The stearyl alcohol (Kalcohl 80, 718) did not increase the reverse mutation rate in histidine dependent bacterial strains of Salmonella typhimurium in the presence or absence of metabolic activation at dose levels determined bu solubility up to 20 ug/plate. There was no evidence of cytotoxicity

**Reliability** : (2) valid with restrictions
Publication, acceptable for assessment.

**Source** : Hachiya, 1982
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

12.08.2005 (8) (23)

## 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Micronucleus assay
**Species** : mouse
**Sex** : male
**Strain** : other: ddY
**Route of admin.** : gavage
**Exposure period** : 24 hours
**Doses** : 360, 730, 1450 mg/kg (single dose) or 730 mg/kg (adminstered 4 times in 24 hours)
**Result** : negative
**Method** : other: mouse bone marrow micronucleus test to protocol to the Japanese Labour Ministry
**Year** : 1982
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Octadecanol (112-92-5) (Kalcohol 80, 718)

**Test condition** : TEST ORGANISMS: Mice
- Age: 6 weeks
- Weight at study initiation: not reported
- No. of animals per dose: Groups of 5 or 6

ADMINISTRATION: Gavage
- Vehicle: Olive oil, dosing volume 25 ml/kg
- Duration of test: 1 or 4 doses.
- Frequency of treatment: Once or 4 times in 24 hours.
- Sampling times and number of samples: 24 hours after a single does, 5 days after the first administraton of the repeated doses. 2000 red blood cells scored per smear for micronuclei, 1000 scored for reticulocytes.
- Control groups and treatment: Stearyl alcohol single oral doses of 0.36, 0.73 or 1.45 g/kg/day or 4 doses of 0.73 g/kg/day in a 24 hour period.

Positive control mitomycin C 3 mg/kg intraperitoneally. Solvent control olive oil 25 ml/kg

EXAMINATIONS:
- Clinical observations: Not reported
- Organs examined at necropsy: Not reported
- Criteria for evaluating results: Not reported
- Criteria for selection of M.T.D.: The maximum single dose was half the LD50. Repeated doses were 1/4 LD50.

STATISTICAL ANALYSIS: Kastenbaum & Bowman

**Result** : MORTALITY: Not reported

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: Not reported

BODY WEIGHT CHANGES: Not reported

FOOD AND WATER CONSUMPTION CHANGES: Not reported

EFFECT ON MITOTIC INDEX OR PCE/NCE RATIO: There were no effects on the incidence of reticulocytes following a single dose of stearyl alcohol. Repeated exposure showed a decrease [controls 61.3%; treated 52.9%]

GENOTOXIC EFFECTS: No significant increase increase in numbers (%) of micronucleated erythrocytes. 10000 - 12000 observed.

NOAEL (NOEL) (C) / LOAEL (LOEL) (C): A single dose of 1450 mg/kg/day or a total repeated dose of 2920 mg/kg did not increase the incidence of micronuclei. There was no reported assessment of effects on the live animals.

**Conclusion** : Stearyl alcohol (Kalcohl 80, 718) did not increase the incidence of micronucleated cells in mouse bone marrow erythrocytes following a single oral dose level up to and including 1450 mg/kg or a total of 2920 mg/kg adminstered as 4 doses in a 24 hour period.

**Reliability** : (2) valid with restrictions
Limited documentation but acceptable for assessment

**Source** : Hachiya et al, 1982
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

12.08.2005 (8) (23)

## 5.7 CARCINOGENITY

**Species** : mouse
**Sex** : no data
**Strain** : other: not stated
**Route of admin.** : other: implantation into the bladder
**Exposure period** : <40 days
**Frequency of treatment** : continuous while the implantation remained intact.
**Post. obs. period** : >290 days
**Doses** : 24-27 mg pellet
**Result** : ambiguous

| | | |
|---|---|---|
| **Control group** | : | yes |
| **Method** | : | other: see below |
| **Year** | : | 1966 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test condition** | : | This study was undertaken to evaluate different substances as possible vehicles for investigation of bladder cancer by implantation.<br><br>TEST ORGANISMS Mice<br>- Age and weight: Not reported.<br>- Number of animals: 56<br><br>ADMINISTRATION / EXPOSURE<br>- Duration of test/exposure: <40 days (the implant disintegrated in this time period)<br>- Type of exposure: Bladder implantation<br>- Post exposure period: >290 days, animals were sacrificed 330 days post implantation.<br>- Dose: Octadecanol was compressed into a pellet weighing 24-27 mg and implanted into the bladder.<br><br>OBSERVATIONS<br>No details given of any routine observations made. Necropsy was carried out 330 days after implantation and histological examination of the bladder carried out. Only animals surviving more than 175 days were evaluated for the presence of bladder carcinomas. Methylcholanthrene implants formed a positive control group.<br><br>ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):<br>The bladder only was examined. |
| **Result** | : | A total of 39 mice died or were killed during the time period of 175 days post implantation to the termination of the experiment (330 days) when the bladder was examined histologically. The average survival time was 308 days. A total of 7 benign tumours and 2 carcinomas developed in the bladders of mice exposed to octadecanol. A low incidence of bladder tumours was observed with all the implants tested. The 20-methyl cholanthrene group showed a high incidence of carcinomas (52%) compared to the octadecanol group (5%) and the other vehicles tested where the carcinoma incidence ranged from 3-17%.<br><br>The authors conclude that any vehicle tested in the form of a pellet implant is likely to be associated with a low incidence of bladder carcinomas. This is probably partly attributable to the pellet acting as a mechanical irritant. No real conclusion on the initiating ptoential of octadecanol can be drawn from this study. |
| **Conclusion** | : | The low incidence of bladder tumours observed following implantation of octadecanol pellets into the bladder of mice is not considered evidence of the carcinogenic potential of ocatadecanol. Various media were implanted in a series of experiments investigating the role of the carrier in bladder tumour development. All implants (including paraffin) produced a low incidence of bladder tumours and mechanical irritation was considered a contributory factor. |
| **Reliability** | : | (2) valid with restrictions<br>Screening test acceptable for assessment |
| **Source** | : | Bryan and Springberg 1966. |

Hayes Consultancy Service Bromley, Kent

| | | |
|---|---|---|
| **Flag** | : | Critical study for SIDS endpoint |
| 12.08.2005 | | (5) |
| **Species** | : | mouse |
| **Sex** | : | female |
| **Strain** | : | Swiss |
| **Route of admin.** | : | dermal |
| **Exposure period** | : | 60 weeks |
| **Frequency of treatment** | : | three times weekly |
| **Post. obs. period** | : | none |
| **Doses** | : | 4 ug/mouse in cyclohexane |
| **Result** | : | negative |
| **Control group** | : | no |
| **Method** | : | other: skin tumour promotion study |
| **Year** | : | 1966 |
| **GLP** | : | no data |
| **Test substance** | : | other TS: Hexanol, Octanol, Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol |
| **Test substance** | : | The substances correspond to C6 through C18 (even carbon number) alcohols CAS RN 111-27-3, 111-87-5, 112-30-1, 112-53-8, 112-72-1, 36653-82-4 and 112-92-5. All have reported purities of about 97%. |
| **Test condition** | : | TEST ORGANISMS<br>- Age/weight: Not reported<br>- Number of animals: 30-50 female swiss mice/group<br><br>ADMINISTRATION / EXPOSURE<br>- Duration of test/exposure: 60 weeks<br>- Type of exposure: dermal (application to shorn dorsal skin) thrice weekly for 60 weeks.<br>- Post exposure period: None<br>- Vehicle: cyclohexane<br>- Concentration in vehicle: 20%<br>- Total volume applied: (1 drop approx. 2ul)<br>- Doses: 4 ug/mouse. Total dose ca 720 mg for each alkanol.<br><br>The mice received a single initiating dose of 7,12-dimethylbenz[a]anthracene in acetone followed one week later by the application (described above) of various alkanols ranging in carbon chain length from C6 to C18, for 60 weeks. Non-initiated groups were included for decanol and dodecanol, these animals received an initial application of acetone alone prior to exposure to the alkanols.<br><br>OBSERVATIONS<br>Skin tumour development was reported and the degree of skin irritation at the application site was assessed. |
| **Result** | : | No skin tumours appeared in the non-initiated groups tested. The incidence of tumour-bearing mice in the initiated groups is as follows:<br><br>hexanol = 0/50<br>octanol = 1/40 (appeared at week 24 and developed into a squamous cell carcinoma)<br>decanol = 6/30 (appeared between weeks 25-36; 2 developed into a squamous cell carcinomas)<br>dodecanol = 2/30 (appeared at week 39 and 49) |

tetradecanol = 2/50 (appeared at week 24 and 26; 1 developed into a squamous cell carcinoma)
hexadecanol = 1/40 (appeared at week 53)
octadecanol = 1/40 (appeared at week 30)

The authors conclude that decanol is a tumour promoting agent and that weak activity is probable with octanol, dodecanol, tetra, hexa and octa decanol. Hexanol was inactive. The authors also note that skin irritation was observed with all the alkanols and was severe with decanol and dodecanol.

**Conclusion** : In this study, published in 1966, the authors conclude that C8-C18 alkanols show some tumour promoting activity with the maximum effect being observed at C10 (decanol). However they also note that skin irritation was present at the application in all of these skin painting experiments with severe irritation being observed with the C10 and C12 alcohols. More recent evidence indicates that irrespective of the causative agent, irritation at the application site is a significant confounder in skin painting studies and its role in the tumour development of non-genotoxic chemicals has been well established (Agyris, 1985, Nessel et al, 1998, 1999).

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Sice 1966.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

12.08.2005 (2) (16) (17) (22)

**Species** : mouse
**Sex** : no data
**Strain** : other: Swiss albino ddY
**Route of admin.** : i.p.
**Exposure period** : 5 days
**Frequency of treatment** : daily
**Post. obs. period** : 24 days
**Doses** : Test 1: 2.5 or 10 mg/mouse/day. Test 2: 2, 4 or 8 mg/mouse/day 2.5 and 10 mg/mouse/day for C16 & 18 alcohols.
**Result** : negative
**Control group** : yes
**Method** : other: determination of antitumour activity against Ehrlichs Ascites Tumour
**Year** : 1972
**GLP** : no
**Test substance** : other TS: other TS: Decanol, Dodecanol, Tetradecanol, Hexadecanol and Octadecanol

**Test condition** : TEST ORGANISMS Mouse Swiss albino ddY implanted ip with ascites tumour cells.
- Age: 5 weeks
- Weight at study initiation: 20-23g
- Number of animals: 4 or 6/ treatment group, 20 controls.

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 5 days starting 24 hours afeter implantation of the ascites tumour cells.
- Type of exposure: Intraperitoneal
- Post exposure period: 24 days
- Vehicle: Probably aqueous suspension using Tween 80.
- Concentration in vehicle: Not reported.

- Doses: Test 1: for all 5 alcohols tested dose levels were 2.5 and 10 mg/mouse. Test 2: C10, 12 and 14 alcohols were tested at 2, 4 and 8 mg/mouse, C16 and 18 alcohols were tested at 2.5 and 10 mg/mouse.

OBSERVATIONS
The mean survival time was recorded and compared to the untreated control group.

**Result** : The C10, 12, and 14 alcohols exhibited toxicity to the mice, evidenced by severe diarrhoea and loss of body weight. The dose levels were reduced in the repeat test. The mean survival time for the untreated control group (Ascites implantation only) was 18.3 days in test1 and 14.4 days in test 2. All of the alkanols tested increased the survival time of mice implanted with ascites tumour cells at one or more dose levels tested. Life span was prolonged by 124 - >194%.

**Conclusion** : Treatment with C10 -18 alcohols extended the survival time of mice implanted intraperitoneally with Ehrlich ascites tumour cells.

**Reliability** : (2) valid with restrictions
Screening test acceptable for assessment

**Source** : Ando et al, 1972
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
12.08.2005 (1)

**Species** : mouse
**Sex** : female
**Strain** : ICR
**Route of admin.** : dermal
**Exposure period** : not reported
**Frequency of treatment** : single application of the initiator 7,12-dimethylbenz[a]anthracene
**Post. obs. period** : Repeated applications of 50:50 1-octadecanol and 1-dodecanol
**Doses** : 125 ug DMBA
**Result** :
**Control group** : no data specified
**Method** : other: tumour promotion study
**Year** : 1974
**GLP** : no
**Test substance** : other TS: 50:50 mixture of 1-octanol and 1-dodecanol

**Test condition** : A mixture of equal parts 1-octadecanol and 1-dodecanol was applied repeatedly (frequency not reported) to the skin of mice which had been initiated with a single application of the carcinogen 7,12-dimethylbenzanthracene.

**Result** : A mixture of 1-octadecanol and 1-dodecanol in equal parts exhibited weak tumour promoting activity at concentrations of 1% or more. When added to Tween 80 there was a moderate reduction in the tumour promoting activity of the Tween 80 particularly at high concentrations (actual concentrations not reported). The is no indication of the degree of irritation observed following the various applications.

**Conclusion** : This study was reported in abstract form only and is included for completeness.

**Reliability** : (4) not assignable
Screening test acceptable for assessment

**Source** : Bock & Tso, 1974

Hayes Consultancy Service Bromley, Kent
12.08.2005 (4)

### 5.8.1 TOXICITY TO FERTILITY

| | | |
|---|---|---|
| **Type** | : | other: Combined repeat dose and Reproductive/Developmental screening study. |
| **Species** | : | rat |
| **Sex** | : | no data |
| **Strain** | : | Wistar |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | males 45 days,up to 54 days |
| **Frequency of treatment** | : | continuous in diet |
| **Premating exposure period** | | |
| **Male** | : | 14 days |
| **Female** | : | 14 days |
| **Duration of test** | : | males 45 days,up to 54 days |
| **Doses** | : | 0, 100, 500, 2000 mg/kg/bw/day |
| **Control group** | : | yes |
| **NOAEL Parental** | : | = 2000 mg/kg bw |
| **NOAEL F1 Offspr.** | : | = 2000 mg/kg bw |
| **Method** | : | other: Combined repeated dose and reproductive/developmental toxicity screening test |
| **Year** | : | 1992 |
| **GLP** | : | yes |
| **Test substance** | : | other TS: Octadecanol (112-92-5) (99% pure) |

**Test condition** :

TEST ORGANISMS: Rat Wistar aged 8 (males) - 9 (females) weeks at start of exposure period. 12M+12F/group

ADMINISTRATION / EXPOSURE
- Type of exposure: Dietary
- Duration of test/exposure: males 45 days, females up to 54 days
- Vehicle: Diet
- Concentration in vehicle: 0, 1500, 7500 & 30,000 ppm

MATING PROCEDURES: 14 day premating exposure, then 1M+1F caged together. Inspection for vaginal plugs thrice daily. If mating did not occur after 14 days cohabitation the female was placed with another male for 8 days.

STANDARDIZATION OF LITTERS: No

PARAMETERS ASSESSED DURING STUDY P:
- Clinical observations: body weight, weight gain, food consumption, food efficiency.
- Estrous cycle: Exposure was for 14 days premating covering at least 2 oestrous cycles. Ovaries were weighed and examined histopathologically at section (5 days after birth).
- Sperm examination: Exposure 14 days premating, no specific sperm analyses carried out, the testes & epididymes were weighed and examined histopathologically.
- Reproductive parameters: Pregancy rate, length of gestation, implantations, corpora lutea and resorptions were recorded.

OFFSPRING: Offspring (and dams) were sacrificed on post natal day 5 and the pups were weighed and examined for external malformations than

sexed and examined for internal malformations.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights P: liver, kidneys, thymus, testis, epididymes.
- Histopathology P: liver, kidneys, adrenals, brain, heart, spleen, ovaries, thymus, testes, epididymides and any organs showing abnormality on macroscopic examination were fixed. The above tissues from all controls and top dose treated rats (except the thymus) plus abnormalities were examined.
- Macroscopic P: Full macroscopic examination.

OTHER EXAMINATIONS: Haematological and biochemical parameters were measured for the Repeat dose toxicity assessment, full details in Chapter 5.4 Repeat dose toxcity

STATISTICAL METHODS: Analysis of variance followed if significant differences were established by Dunnetts T-test to assess possible intergroup differences. For pregnancy rate a Qui2-test was carried out to confirm lack of significance.

**Result** **:** NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 500 and 2000 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Parental data and F1:
- Body weight: No treatment related effects.
- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.
- Pregancy rate: There was no statistically significant difference in pregnancy rates (confirmed using a Qui2-test) although they were reduced in treated groups C 92%, 100 & 500 mg/kg 75%, 2000 mg/kg/day 67% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams (mean 22 days for all groups).
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Effects on sperm: Not reported
- Clinical biochemistry findings incidence and severity: (males only investigated) None considered of biological significance see Chapter 5.4 Repeated dose toxicity for fuller details.
- Haematological findings incidence and severity: (males only investigated) The significance of changes in plasma free cholesterol, triglycerides and glucose is unclear, the changes were observed at all doses levels but were not dose related. They may be related to differences in dietary composition. See Chapter 5.4 Repeated dose toxicity for fuller details.
- Organ weights: There were no statistically significant dose related changes in organ weights including the testes, epididymes and ovaries.
- Gross pathology: There were no changes attributable to exposure to the test compound.
- Histopathology: There were no treatment related histopathological

changes including no effects in the testes and ovaries.
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups )Mean 13 in controls and low dose, 15 in mid and high dose groups). Resorptions mean for controls and low dose 0, for mid and high dose 1).
- Number of corpora lutea: No significant differences between treated and control groups (mean controls 13, low and mid dose 14, high dose 15).
- Ovarian primordial follicle counts: Not reported
- Offspring toxicity F1:
- Litter size and weights: No effect of treatment (mean liter size 11.73, 10.0, 13.6 and 13.38 for controls, low, mid and high dose respectively).
Letter weights day 1 mean 69, 61, 75 and 75 gm; Day 4 mean 96, 84, 101 and 101gm for controls, low, mid and high dose respectively)
- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.

**Conclusion** : Parental NOAEL 2000 mg/kg/day changes in plasma free cholesterol, triglycerides and glucose were observed at all doses levels but were not dose related and may be due to differences in dietary composition. There were no statistically significant adverse effects on reproductive parameters and the NOAEL for reproductive and developmental effects can be considered as 2000 mg/kg/day (highest dose level).

**Reliability** : (2) valid with restrictions
Comparable to guideline study (draft guideline) with acceptable restrictions
**Source** : Hansen 1992b.
Hayes Consultancy Service Bromley, Kent
**Flag** : Critical study for SIDS endpoint
08.01.2006 (9)

**Type** : other: Repeat dose study with histopathology of reproductive organs.
**Species** : rat
**Sex** : male/female
**Strain** : Sprague-Dawley
**Route of admin.** : gavage
**Exposure period** : 28 days
**Frequency of treatment** : daily 5 days/week
**Premating exposure period**
**Male** :
**Female** :
**Duration of test** :
**Doses** : 0, 100, 500, and 1000 mg/kg in olive oil
**Control group** : yes
**NOAEL Parental** : = 1000 mg/kg bw
**Method** : other: OECD Guideline 407
**Year** : 1996
**GLP** : yes
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : Tradename Lanette 18

**Test condition** : Groups of 10M+10F rats received daily doses of 0, 100, 500 and 1000 mg/kd Lanette 18 by gavage for 28 days. Full details of this study are reported in Chapter 5.4 Repeated dose toxicity. The testes and ovaries were weighed and these organs plus the prostate and uterus from all control and top dose animals were subject to histopathological examination.

| | | |
|---|---|---|
| **Result** | : | No animals died during the test. Food intake and water consumption were comparable to the control group. Body weight gain and total increase of body weights did not differ from control values. There were no significant differences in the weight of the testes or ovaries. Histopathological examination of the testes, prostate, ovaries and uterus revealed no treatment related changes. NOAEL for effects on the reproductive organs 1000 mg/kg/day. |
| **Reliability** | : | (1) valid without restriction<br>Guideline study |
| **Source** | : | Henkel KGaA 1986a<br><br>Hayes Consultancy Service Bromley, Kent |

12.08.2005 (13) (14)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Wistar |
| **Route of admin.** | : | oral feed |
| **Exposure period** | : | Up to 54 days, premating, mating and gestation until post natal day 5. |
| **Frequency of treatment** | : | continuous in diet |
| **Duration of test** | : | Up to 54 days |
| **Doses** | : | 0, 100, 500, 2000 mg/kg/bw/day |
| **Control group** | : | yes |
| **NOAEL Maternalt.** | : | = 2000 mg/kg bw |
| **NOAEL Teratogen** | : | = 2000 mg/kg bw |
| **Method** | : | other: Combined repeat dose and reproductive/developmental toxicity screening test |
| **Year** | : | 1992 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | Octadecanol (112-92-5) Purity 99% |
| **Test condition** | : | Groups 12 female rats were given otadecanol in the diet at doses of 0, 1500 ppm, 7500 ppm, and 30000 ppm (0, 100, 500 and 2000 mg/kg/day) for a period of 14 days prior to mating then throughout mating and gestation until post natal day 5 when dams and offspring were sacrificed. This is part of a combined repeat dose and reproductive/developmental screening study (similar to OECD 422). Reproductive parameters examined were pregancy rate, length of gestation, implantations, corpora lutea and resorptions. On post natal day 5 the pups were weighed and examined macroscopically for external malformations then sexed and examined for internal malformations. For full details of this study see chapter 5.4 Repeated dose toxicity and chapter 5.8.1 Fertility. |
| **Result** | : | NOAEL: 2000 mg/kg/day (highest dose tested) for systemic and reproductive toxicity.<br><br>ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: ca 100, 500 and 2000 mg/kg/day<br><br>TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:<br>- Parental data:<br>- Body weight: No treatment related effects. |

- Food/water consumption: No treatment related effects.
- Description, severity, time of onset and duration of clinical signs: None reported.
- Pregnancy rate: There was no statistically significant difference (confirmed using a Qui2-test) in pregnancy rates although they were reduced in treated groups C 92%, 100 & 500 mg/kg 75%, 2000 mg/kg/day 67% these were within the normal historical control range according to the authors (actual historical control data not presented).
- Fertility index: Not reported
- Precoital interval: Not reported
- Duration of gestation: Comparable in treated and control dams.
- Gestation index: Not reported
- Changes in lactation: Not reported
- Changes in estrus cycles: Not reported
- Mortality: None
- Number of implantations: No significant differences in the numbers of implantations between treated and control groups. (Mean 13 in controls and low dose, 15 in mid and high dose groups). Resorptions mean for controls and low dose 0, for mid and high dose 1)..
- Number of corpora lutea: No significant differences between treated and control groups (mean controls 13, low and mid dose 14, high dose 15).
- Ovarian primordial follicle counts: Not reported
- Foetal toxicity:
- Litter size and weights: No effect of treatment. (mean litter size 11.73, 10.0, 13.6 and 13.38 for controls, low, mid and high dose respectively). Litter weights day 1 mean 69, 61, 75 and 75 gm; Day 4 mean 96, 84, 101 and 101gm for controls, low, mid and high dose respectively)

- Sex and sex ratios: No treatment related effects.
- Post natal survival until day 5: Similar in treated and control groups.
- Foetal anomalies: There were no treatment related changes in the incidence of external or visceral malformations visible on macroscopic examination.

**Conclusion** : Development was assessed as part of a combined repeat dose and reproductive/developmental toxicity study. There were no adverse effects on maternal toxicity or reproductive parameters and no adverse effect on the offspring which were examined on postnatal day 5. The NOAEL for maternal and foetotoxicity in rats, receiving octadecanol in the diet for up to 54 days (premating, mating, gestation until postnatal day 5), was 2000 mg/kg/day (highest dose level). There was no evidence of teratogenicity from the limited examinations of the pups which were carried out.

**Reliability** : (1) valid without restriction
Comparable to guideline study (draft guideline) with acceptable restrictions

**Source** : Hansen 1992b.
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint

08.01.2006 (9)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

**Remark** : The purpose of this study was to compare the nitrocellulose-replica method (24 hour semi-occlusive exposure to the flexor surface of the arms) with closed patch testing (24 hour application to the back in a Finn chamber, 15 ul test material). The study was based on 20 healthy volunteers.

The results evaluated using the closed patch testing showed that skin irritation for octanol significantly increased with increasing concentration of the test compound. Lauryl, cetyl and stearyl alcohols were of low irritancy. However the nitrocellulose-replica method could detect skin irritation with the higher alcohols which was not observed in the closed patch testing.

**Source** : Sato et al, 1996
Hayes Consultancy Service Bromley, Kent

**Test substance** : octyl alcohol, lauryl alcohol, cetyl alcohol, stearyl alcohol.

**Reliability** : (2) valid with restrictions

06.09.2004 (20)

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# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

| | | |
|---|---|---|
| | : | **HYDROFORMYLATION PRODUCTS** |
| **CAS No.** | : | 68516-18-7, 68527-05-9, 70955-11-2 and preparations containing mixtures of these products |
| **EINECS Name** | : | Decene, hydroformylation products, Octene, hydroformylation products, Hexene, hydroformylation products and preparations containing mixtures of these products |
| **EC No.** | : | - |
| **Molecular Formula** | : | - |

# AQUATIC ORGANISMS

## 4.1 Acute/Prolonged Toxicity to Fish

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 3.2
**LC50:** = 10
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 7900

**Result:** RESULTS: EXPOSED
NOEC = 3.2 mg/l
EC50 = 10 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: 0

Abnormal effects such as surfacing, dark discoloration and fish resting on the bottom of test chambers were observed in the 10 and 5.6 mg/l test chambers. After 24 hours, 50% mortality had occured in the 10 mg/l test chamber and 100% mortality had occured in the 18 and 32 mg/l concentrations.
**Source:** Cohle and McAllister 1983a.
**Test condition:** TEST ORGANISMS
Strain: Salmo gairdneri
Supplier: Trout Lodge; McMillan, Washington
Age: Not reported
Weight: mean 0.33g
Feeding: Standard commercial fish food (Rangen's) daily
Pretreatment: Observed for 14 days prior to testing
Feeding during test: Not reported
Control group: Dilution water control and solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle, solvent: 3.2 ml in highest test concentration and solvent control
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: ABC laboratory well water
Aeration: Not reported
Alkalinity: 368 ppm CaCo3
Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: ranging from 3.2-32 mg/l in a logarithmic series
Exposure vessel type: 15 gallon glass vessel
Number of replicates: 1
Fish per replicate: 10
Test temperature: 12 C

Dissolved oxygen: 8.7 - 9.6 mg/l
pH mean: 8.1
Adjustment of pH: none
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: lethality
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Test substance:** This substance corresponds to a mixture of 58% Octene hydroformylation products (68527-05-9) and 40% Hexene hydroformylation products (70955-11-2), C 7:9, 40:58%.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

10-SEP-2003 (5)

**Type:** static
**Species:** Lepomis macrochirus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 10
**LC50:** = 13
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 7900

**Remark:** The study was conducted at nominal concentrations of 5.6, 10, 18, 32 and 56 mg/l. Acetone was used as the solvent. Ten fish were exposed to each concentration. There were no deaths in the control or solvent group.

**Source:** Cohle and McAllister 1983b.

**Test substance:** This substance corresponds to a mixture of 58% Octene hydroformulation products (68527-05-9) and 40% Hexene hydroformulation products (70955-11-2), C 7:9, 40:58%.

**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available

18-AUG-2003 (6)

**Type:** static
**Species:** Salmo gairdneri (Fish, estuary, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 1.8
**LC50:** = 8
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 7911

**Result:** RESULTS: EXPOSED
NOEC = 1.8 mg/l
EC50 = 8 mg/l
Based on nominal concentration
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Cohle and McAllister 1983c.
**Test condition:** TEST ORGANISMS
Strain: Salmo gairdneri
Supplier: Trout Lodge, McMillan, Washington
Age: Not reported
Weight: 1.1g
Feeding: Standard commercial fish food (Rangen's) daily
Pretreatment: Acclimated for 48 hours in the dilution water and held without food
Feeding during test: not reported
Control group: Dilution water control and solvent control group
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle/solvent: 10 ml in highest test concentration and solvent control
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: ABC laboratory well water
Aeration: Not reported
Alkalinity: 368 ppm CaCO3
Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: 1.0, 1.8, 3.2, 5.6, and 10 mg/l
Exposure vessel type: 5 gallon glass vessels
Number of replicates: not reported
Fish per replicate: 10
Test temperature: 12 C
Dissolved oxygen: 6.1-9.3 mg/l
pH mean: 8.0-8.2
Adjustment of pH: None
Intensity of irradiation: Not reported
Photoperiod: Not reported
TEST PARAMETER: lethality
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported
**Test substance:** This substance is a mixture and corresponds to 33% each of Decene (68516-18-7), Octene (68527-05-9), and Hexene (70955-11-2) hydroformylation products.
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
19-AUG-2003 (7)

**Type:** static
**Species:** Lepomis macrochirus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 3.2
**LC50:** = 8.8
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 7911

**Result:** Mortality was accompanied by effects such as loss of equilibrium, quiescence, dark discoloration, and fish resting on the bottom of the test chambers.

**Source:** Cohle and McAllister 1983d.
**Test condition:** The study was conducted at nominal concentrations of 3.2, 5.6, 10, 18 and 32 mg/l. Ten fish, with a mean weight of 0.52 g and a mean length of 29 mm were exposed to each test concentration and control.
**Test substance:** This substance is a mixture and corresponds to 33% each of Decene (68516-18-7), Octene (68527-05-9), and Hexene (70955-11-2) hydroformylation products.
**Reliability:** (2) valid with restrictions
Not key study: Other studies (same reliability score) showing greater toxicity are available
19-AUG-2003 (8)

**Type:** static
**Species:** Lepomis macrochirus (Fish, fresh water)
**Exposure period:** 96 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 1.8
**LC50:** = 3.8
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 1100

**Result:** RESULTS: EXPOSED
NOEC = 1.8 mg/l
LC50 = 3.8 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0
**Source:** Burgess and Forbis 1983a.
**Test condition:** TEST ORGANISMS
Strain: Lepomis macrochirus
Supplier: Osage Catfisheries, Osage Beach, Missouri
Age: Not reported
Weight: 0.16 g
Feeding: Standard commercial fish food (Rangen's)
Pretreatment: Acclimatised to test conditions for 48 h prior to testing
Feeding during test: Discontinued 48 h prior to testing
Control group: Dilution water control and solvent control chamber
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: acetone
Concentration of vehicle/solvent: 5 ml in highest test concentration and solvent control group
STABILITY OF TEST CHEMICAL SOLUTIONS
not reported
DILUTION WATER
Source: ABC laboratory well water
Aeration: Not reported
Alkalinity: 368 ppm CaCO3
Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: 1.0, 1.8, 3.2, 5.6, 10 mg/l
Renewal of test solution: not reported

Exposure vessel type: 5 gallon glass vessels
Number of replicates: not reported
Fish per replicate: 10
Test temperature: 22 C
Dissolved oxygen: 6.0-8.8 mg/l
pH mean: 7.9-8.3
TEST PARAMETER: mortality
MONITORING OF TEST SUBSTANCE CONCENTRATION: not reported

**Test substance:** This substance corresponds to Decene hydroformylation products, CAS #68516-18-7.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

23-MAR-2004 (1)

## 4.2 Acute Toxicity to Aquatic Invertebrates

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**NOEC:** = 5.6
**LC50 :** = 11
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: C7-C11 alcohols

**Result:** RESULTS: EXPOSED
LC50 11 (5.6-18) mg/l
NOEC 5.6 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Burgess and Forbis 1983d.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: ABC Laboratory
Age: < 24hrs old
Feeding: Selenastrum capricornutum and trout chow
Pretreatment: Not reported
Feeding during test: No feeding during test
Control group: Control and solvent group (Solvent control received an aliquot 0.56 ml of acetone equivalent to that of the highest concentration)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: Not reported
STABILITY OF THE TEST CHEMICAL SOLUTIONS: No analysis
DILUTION WATER
Source: Well water
Aeration: Not reported
Alkalinity: 368 ppm CaCO3
Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: 5.6, 10, 18, 32, and 56 mg/l
Renewal of test solution: None

Exposure vessel type: 250 ml glass beaker
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 21 C
Dissolved oxygen: 7.3 - 7.7 mg/l
pH mean: 8.3 - 8.6
Adjustment of pH: not reported
Intensity of irradiation: 50-70 foot candles (540-750 lux)
Photoperiod: 50-70 foot candles 16 hour daylight
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:
Not reported

**Test substance:** This substance is a mixture and corresponds to 33% each of Decene (68516-18-7), Octene (68527-05-9), and Hexene (70955-11-2) hydroformylation products. Tradename is Oxo alcohol 7911.

**Reliability:** (2) valid with restrictions
Test substance concentration analysis was not carried out during the test.

**Flag:** Critical study for SIDS endpoint

14-AUG-2003 (4)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 30
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 7900

**Result:** RESULTS: EXPOSED
LC50 = 30 mg/l
NOEC = 10 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Burgess and Forbis 1983c.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: ABC Laboratory
Age: < 24hrs old
Feeding: Selenastrum capricornutum and trout chow
Pretreatment: Not reported
Feeding during test: Not reported
Control group: Control and Solvent group (Solvent control received an aliquot 0.56 ml of acetone equivalent to that of the highest concentration)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: 0.028% to 0.28%
STABILITY OF THE TEST CHEMICAL SOLUTIONS: No analysis
DILUTION WATER
Source: Well water
Aeration: Not reported
Alkalinity: 368 ppm CaCO3

Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: 5.6, 10, 18, 32, and 56 mg/l, Control with solvent and Control
Renewal of test solution: None
Exposure vessel type: 250 ml glass beaker
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 21 C
Dissolved oxygen: 7.3 - 7.7 mg/l
pH mean: 8.3 - 8.6
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: 50-70 foot candles 16 hour daylight
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:
None

**Test substance:** This substance is a mixture and corresponds to 58% octene hydroformylation products (68527-05-9) and 40% hexene hydroformylation products (70955-11-2).

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

11-SEP-2003 (3)

**Type:** static
**Species:** Daphnia magna (Crustacea)
**Exposure period:** 48 hour(s)
**Unit:** mg/l **Analytical monitoring:** no data
**LC50 :** = 4.2
**Limit Test:** no

**Method:** other: EPA 660/3-75-009; APHA 1975.
**Year:** 1983
**GLP:** yes
**Test substance:** other TS: Oxo alcohol 1100

**Result:** RESULTS: EXPOSED
LC50 = 4.2 mg/l
NOEC = 1.8 mg/l
Based on nominal concentrations
RESULTS: CONTROL
Number/% showing adverse effects: 0

**Source:** Burgess and Forbis 1983b.

**Test condition:** TEST ORGANISMS
Strain: Daphnia magna
Supplier: ABC Laboratory
Age: < 24hrs old
Feeding: Selenastrum capricornutum and trout chow
Pretreatment: Not reported
Feeding during test: Not reported
Control group: Control and solvent group (Solvent control received an aliquot 0.18 ml of acetone equivalent to that of the highest concentration)
STOCK AND TEST SOLUTION AND THEIR PREPARATION
Vehicle, solvent: Acetone
Concentration of vehicle, solvent: Not reported
STABILITY OF THE TEST CHEMICAL SOLUTIONS: No analysis
DILUTION WATER

Source: Well water
Aeration: Not reported
Alkalinity: 368 ppm CaCO3
Hardness: 255 ppm CaCO3
Conductance: 500 umhos/cm
TEST SYSTEM
Concentrations: 1.8, 3.2, 5.6, 10, and 18 mg/l, Control with solvent and Control
Renewal of test solution: None
Exposure vessel type: 250 ml glass beaker
Number of replicates: 2
Invertebrate per replicate: 10
Test temperature: 21 C
Dissolved oxygen: 8.1 - 8.2 mg/l
pH mean: 8.3
Adjustment of pH: not reported
Intensity of irradiation: not reported
Photoperiod: 50-70 foot candles 16 hour daylight
TEST PARAMETER: Mortality/immobility
MONITORING OF TEST SUBSTANCE CONCENTRATION:
None

**Test substance:** This substance corresponds to Decene hydroformylation products, CAS # 68516-18-7.

**Reliability:** (2) valid with restrictions

**Flag:** Critical study for SIDS endpoint

12-MAR-2004 (2)

(1) Burgess, D. and Forbis, A.D. 1983a. Acute toxicity of oxo alcohol 1100 to Bluegill Sunfish (Lepomis macrochirus). Static bioassay report 30849.

(2) Burgess, D. and Forbis, A.D. 1983b. Acute toxicity of oxo alcohol 1100 to Daphnia magna. Static acute bioassay report 30851.

(3) Burgess, D. and Forbis, A.D. 1983c. Acute toxicity of oxo alcohol 7900 to Daphnia magna. Static acute bioassay report 30845.

(4) Burgess, D. and Forbis, A.D. 1983d. Acute toxicity of oxo alcohol 7911 to Daphnia magna. Static acute bioassay report 30848.

(5) Cohle, P.R. and McAllister, W.A. 1983a. Acute toxicity of oxo alcohol 7900 to Rainbow Trout (Salmo gairdneri). Static bioassay report 30844.

(6) Cohle, P.R. and McAllister, W.A. 1983b. Acute toxicity of oxo alcohol 7900 to Bluegill Sunfish (Lepomis macrochirus). Static bioassay report 30843.

(7) Cohle, P.R. and McAllister, W.A. 1983c. Acute toxicity of oxo alcohol 7911 to Rainbow Trout (Salmo gairdneri). Static bioassay report 30847.

(8) Cohle, P.R. and McAllister, W.A. 1983d. Acute toxicity of oxo alcohol 7911 to Bluegill Sunfish (Lepomis macrochirus). Static bioassay report 30846.

# SUPPORTING ROBUST SUMMARIES

# Long Chain Aliphatic Alcohols category

**Note: This file contains robust summaries for key supporting data only, and is not a complete SIDS Dossier. No attempt has been made to fill data gaps. Data are used for validation purposes only, and are presented in the SIAR as needed.**

**Please refer to section 1 of the SIAR for a discussion of the role of supporting substances.**

| | | |
|---|---|---|
| **Existing Chemical** | **:** | ID: 123607-66-9 |
| **CAS No.** | **:** | 123607-66-9 |

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

**In Vitro/in vivo** : In vivo
**Type** : Distribution
**Species** : rat
**Number of animals**
**Males** : 12
**Females** :
**Doses**
**Males** : 10 uCi [8-(C14)]-octacosanol
**Females** :
**Vehicle** : other: tricaproyl glycerol
**Route of administration** : gavage
**Exposure time** : 7 day(s)
**Product type guidance** :
**Decision on results on acute tox. tests** :
**Adverse effects on prolonged exposure** :
**Half-lives** : 1st.:
2nd.:
3rd.:
**Toxic behaviour** :
**Deg. product** :
**Method** :
**Year** : 1993
**GLP** : no data
**Test substance** : other TS: octacosanol
**Test condition** : The rats received a single oral dose of 10 uCi [8- C14]-octacosanol. 3 animals were sacrificed at each of th efollowing time points 1,2,3 and 7 days. Samples of blood, liver, kidneys, lungs, brain, spleen, GI tract, adipose tissue and muscle were taken for analysis. Expired air and excreta were collected from each animal indivdually over a 7 day period for anialysis of radioactivity inexpired air, urine and faeces.

**Result** : Disposition: The highest concentration of plasma radioactivity was reached in 1 hour indicating rapid abosroption. The presence of radioactivity in the various organs was low the highest concentration being observed in the liver. The highest concentration over all was found in the adipose tissues.

Excretion: Excretion via the faeces was about 32% of the administered dose, 26% being excreted within 24 hours. Urinary excretion was very small in comparison. Expiration of radioactive CO2 over 7 days accounted for 15% of the dose administered, with 50% occurring in the first 24 hours.

The excretion of radioactivity via urine, faeces and expired air over the 7 days was ca 49% of the dose administered. Total recovery was 32.14% in the faeces, 1.31% in the urine and 15.12% in expired CO2.

Metabolites: chloroform methanol (2:1) extractions of the urine and faeces were prepared. Faecal radioactivity was almost entirely extracted by the solvent while urinary radioactivity was mainly present in the water layer. This suggests that the faecal radioactivity might be due to unchanged octacosanol while the urinary radioactivity might be due to metabolites however these were not identified.

**Reliability** : (2) valid with restrictions
Publication, study fairly well documented, meets generally accepted scientific principles, acceptable for assessment.

17.06.2005 (2)

**In Vitro/in vivo** : In vivo
**Type** : Distribution

**Species** : rat
**Number of animals**
**Males** :
**Females** :
**Doses**
**Males** : 2.0 uCi/dose of (8-14C)-octacosanol
**Females** :
**Vehicle** :
**Route of administration** : gavage
**Exposure time** :
**Product type guidance** :
**Decision on results on acute tox. tests** :
**Adverse effects on prolonged exposure** :
**Half-lives** : 1st.:
2nd.:
3rd.:
**Toxic behaviour** :
**Deg. product** :
**Method** :
**Year** : 1995
**GLP** : no data
**Test substance** : other TS: octacosanol

**Test condition** : Male wistar rats aged 4 weeks received repeated doses of 14C-octacosanol twice daily at 10 hour intervals for a total of 2, 6 or 10 doses. The animals were sacrificed 12 hours after the last dose. 3 animals were sacrificed for each dose except after 10 doses when one animal only was sacrificed.

In another experiment administration was carried out as above but terminated after 9 doses and the animals sacrificed after 1, 3, 4 or 9 days. In this these animals whole body autoradiography was carried out after 1 and 4 days. An adjacent section of each organ in the autoradiograph sections was taken to calculate the mean exposed radioactivity of the section.

Samples of aortic blood, liver, kidney, spleen, heart, lungs, brain, GI tract and adipose tissue were taken at each sacrifice time. Faeces were collected separately each day for the duration of the experiment.

**Result** : When expressed per organ the highest amount of radioactivity was found in the liver (9.5% of administered dose) followed by the GI tract (8.2%) and muscle (3.5%) at all doses. Levels of radioactivity in other tissues were minimal (<0.9%). Liver radioactivity diminished rapidly after the 2-dose administration even when the doses were increased. Muscles however appeared to accumulate radioactivity. In the 9 daose series after 3 and 9 days the accumulation of radioactivity was higher in the muscles than in the liver. Plasma radioactivity reached a peak when liver and muscle activity was low (after 6 or 10 doses). It appears that the tissues become saturated after administration of 2 doses and subsequent doses do not result in increased uptake.

Plasm activity and faecal excretion reached a maximum on the 3rd day of the 6 doses. Excretion in the faeces was almost constant at a level of 21-25% of administered dose at all doses investigated. The cumulative excretion of radioactivity in the rat faeces was 31 and 33% of dose after 3 and 9 days in the 9-dose serial administration.

The autoradiographs showed that a significant amount of radioactivity was trapped in blood (0.33% of dose/ml), skin (0.44%/g), bones (0.30%/g) and

other tissues.

**Reliability** : (2) valid with restrictions
Publication, study fairly well documented, meets generally accepted scientific principles, acceptable for assessment.

17.06.2005 (4)

**In Vitro/in vivo** : In vivo
**Type** : Metabolism
**Species** : rat
**Number of animals**
**Males** : 24
**Females** :
**Doses**
**Males** : 2.0 uCi/dose of (8-14C)-octacosanol
**Females** :
**Vehicle** : other: tricaproyl glycerol
**Route of administration** : gavage
**Exposure time** :
**Product type guidance** :
**Decision on results on acute tox. tests** :
**Adverse effects on prolonged exposure** :
**Half-lives** : 1st:
2nd:
3rd:
**Toxic behaviour** :
**Deg. product** :
**Method** : other
**Year** : 1995
**GLP** : no data
**Test substance** : other TS: octacosanol

**Test condition** : Groups of 3 male Wistar rats received a single 2.0 uCi/dose of (8-14C)-octacosanol in tricaproyl glycerol. The animals were sacrificed at 0.5, 1, 2, 4, 6, 8, 10 and 24 hour intervals after dosing.

Aortic blood was taken on sacrifice, samples of liver, kidneys, spleen, heart, lungs gastroinestinal tract and a portion of leg muscle were taken at all time periods. Liver parameters were investigated after 4 hours (total lipid and lipid fractionation). Expired CO2, urine and faeces were collected at radioactivity measrued at 24 hours.

**Result** : In the first 30 minutes following oral administration uptake by the liver and muscle was low (0.08 and 0.26% of administered dose respectively) this increased markedly to 2.6-2.7%) between 4-6 hours in the liver and to 1.8% at 8 hours in the muscles. This was followed by a decrease to approx 1% in both tissues at 24 hours. Over this time period levels in other tissues investigated were <0.05%.

Of the radioactivity in the liver at 4 hours 36.2% was recovered in the sterol fraction, 19.5% in the phospholipid fraction and 3.4% in the triglyceride fraction. This was interpreted to indicate conversion of the fatty alcohol into acid followed by incorporation into phospholipids and sterols. This is supported by the detection of radioactivity in the expired CO2 (2.3% of absorbed radioactivity) at this time period.

**Reliability** : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

10.08.2005 (3)

### 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Species** | : | rat |
| **Strain** | : | Sprague-Dawley |
| **Sex** | : | male/female |
| **Number of animals** | : | 80 |
| **Vehicle** | : | other: gum arabic - water suspension |
| **Value** | : | > 5000 mg/kg bw |
| **Method** | : | other |
| **Year** | : | 1995 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test condition** :

TEST ORGANISMS: Rat, Sprague-Dawley
- Source: National Centre for the Production of Laboratory Animals, Cuba
- Age: Not reported
- Weight at study initiation: 150 - 200g
- Group size: 8 males + 8 females per group
- Controls: Yes, vehicle only

ADMINISTRATION: Oral
- Doses: 0, 500, 1500, 2500 and 5000 mg/kg
- Doses per time period: single
- Volume administered or concentration: Animals received similar volumes of the vehicle.
- Vehicle: 10 mg/ml gum arabic in water.
- Post dose observation period: 14 days

EXAMINATIONS: Observations of clinical signs were made hourly in the first 4 hours after dosing, 4 hourly thereafter to 24 hours and then daily. Bodyweights were recorded at the start and finish of the experiment. At the end of the observation period, blood samples were taken for haematological and biochemical analyses of haemoglobin, haematocrit, GOT amd GPT, alkaline phosphatase, creatinine and glucose. All animals were subject to gross histopathological examination and organ weights (liver, kidneys, heart, spleen, lungs and thymus) were recorded. Histopathological examination was carried out on all top dose and control rats.

STATISTICAL ANALYSIS: Biochemical and haematological parameters and organ weights were analysed using variance analysis (ANOVA) and carried out independently for each sex. Analysis of mortality and frequency of histopathological signs were conducting using the Fischer Exact Proportions TEst.

**Result** :

MORTALITY:
- Time of death: All rats survived the 14 day observation period. LD50 >5000 mg/kg

CLINICAL SIGNS: There were no signs of toxicity. Increase in bodyweight was similar between treated and control groups and there were no statistical differences.

HAEMATOGLOGY AND BIOCHEMISTRY: No statistically significant changes attributable to treatment.

NECROPSY FINDINGS: No remarkable changes in gross or microscopic pathology. No significant changes in the weight of the major organs

weighed.

POTENTIAL TARGET ORGANS: None identified

SEX-SPECIFIC DIFFERENCES: None identified

**Conclusion** : The rat oral LD50 for sample D-002 is >5000 mg/kg. There were no mortalities or other adverse effects on any of the parameters monitored.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail.

**Flag** : Critical study for SIDS endpoint
10.08.2005 (5)

**Method** :
**Year** :
**GLP** :
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : Unpublished data provided by Rodeiro, 1996 giving LD50 values in mice, rabbits and dogs. All three species showed no measurable toxicity at dose levels of up to 5000 mg/kg.

**Reliability** : (4) not assignable
Citation of unpublished results, no further details available.
11.04.2005 (8)

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

**Species** : dog
**Sex** : male/female
**Strain** : Beagle
**Route of admin.** : gavage

| | | |
|---|---|---|
| **Exposure period** | : | 1 year |
| **Frequency of treatment** | : | daily, 7 days/week |
| **Post obs. period** | : | none |
| **Doses** | : | 50, 250 mg/kg bw |
| **Control group** | : | yes |
| **NOAEL** | : | = 250 mg/kg bw |
| **Method** | : | other |
| **Year** | : | 2001 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%
octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

**Test condition** : TEST ORGANISMS
- Age: 10-12 weeks
- Weight at study initiation: 8-12 kg
- Number of animals: 4M+4F per group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 1 year
- Type of exposure: oral gavage
- Post exposure period: none
- Vehicle: 1% acacia gum in water
- Concentration in vehicle: Varied according to dose level.
- Total volume applied: 8 ml/kg
- Doses: 0, 50, 250 mg/kg/day (250 mg/kg/day was the highest level which could be given in a single dose because of solubility considerations)

SATELLITE GROUPS AND REASONS THEY WERE ADDED:

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Monthly
- Food consumption: Daily
- Water consumption: Not recorded
- Ophthalmoscopic examination: None
- Haematology: Venous blood prestudy and at 3 monthly intervals. Hb & heamatocrit only were determined.
- Biochemistry: Venous blood prestudy and at 3 monthly intervals. glucose, aspartate and alanine transferases, creatinine and acetyl cholinesterase.
- Urinalysis: Not done.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Full necropsy.
- Organ weights: Liver, kidneys, heart, lungs, spleen, thymus, adrenals, testis, prostate (not ovaries)
- Microscopic: All major organs including gonads.

STATISTICAL METHODS: Body weight, organ weight and blood parameters were analysed with a variance analysis (Kruskall-Wallis non-parametric ANOVA test). Histopathological results were compared using Fischers exact test. P<0.05 was established for statistical significance.

**Result** : NOAEL (NOEL): 250 mg/kg/day (highest dose level tested)

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 0, 50 and 250 mg/kg/day

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: None
- Clinical signs: None
- Body weight gain: No significant differences between treated and control groups.
- Food consumption: Not reported.
- Clinical chemistry: No significant differences.
- Haematology: No significant differences.
- Organ weights: No significant differences.
- Gross pathology: Normal
- Histopathology: No treatment related changes. Autoimmune thyroiditis was observed in one control female. 1 treated male dog at each dose level also showed this type of lesion associated with adenitis. Particular attention was paid to examination of the stomach as a target organ for anti-ulcer drug toxicity (D-002 is used as an anti-ulcer drug). There was no evidence of any damage to the gastric mucosa.

**Conclusion** : NOAEL 250 mg/kg/day (highest dose level tested). No treatment related adverse effects were observed in this study which included histopathological examination of the male and female reproductive organs.

**Reliability** : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Aleman 2001.
Hayes Consultancy Service Bromley, Kent

24.01.2005 (1)

**Species** : rat
**Sex** : male/female
**Strain** : Sprague-Dawley
**Route of admin.** : gavage
**Exposure period** : 14 days
**Frequency of treatment** : daily
**Post obs. period** : none
**Doses** : 2000, 3000, 5000 mg/kg/day
**Control group** : no data specified
**NOAEL** : > 5000 mg/kg bw
**Method** : other: screening
**Year** : 1998
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%

octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

**Test condition** : The test material D-002 was prepared as a suspension in acicia gum/water (10 mg/ml). Groups of 5M+5F rats reeceived daily doses of 2000, 3000 or 5000 mg/kg for 14 dyas. Clinicals signs were observed regualrly and body weights recorded prior to the first treatment then at 7 and 14 days. Biochemical determinations and histopathological examination was carried out at the end of the study.

**Result** : There were no adverse effects on any of th eparameters studied. The 14 day LD50 was >5000 mg/kg.

**Reliability** : (2) valid with restrictions
16.05.2005 (7)

**Species** : rat
**Sex** : male/female
**Strain** : Sprague-Dawley
**Route of admin.** : gavage
**Exposure period** : 90 days
**Frequency of treatment** : daily
**Post obs. period** : none
**Doses** : 0, 5, 25, 125, 625 mg/kg/day
**Control group** : yes
**NOAEL** : > 625 mg/kg bw
**Method** : other:
**Year** : 1998
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test substance** : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%
octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

**Test condition** : TEST ORGANISMS SD rats
- Age: 6-8 weeks
- Weight at study initiation: 150-200 g
- Number of animals: 12M+12F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 90 days
- Type of exposure: gavage
- Post exposure period: none
- Vehicle: As a suspenson in acacia gum/water
- Concentration in vehicle: 10 mg/ml
- Doses: 0, 5, 25, 125, 625 mg/kg/day

SATELLITE GROUPS AND REASONS THEY WERE ADDED: None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: No data
- Haematology: Haemoglobin, Haematocrit, total and differential white cell count.
- Biochemistry: At the end of the assay. ALAT, ASAT, creatininte, acetyl cholinesterase, alkaline phosphatases, creatin-kinase, urea.
- Urinalysis: No

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Organ weights are reported for liver, kidney, Heart, Lungs, Spleen and Thymus, organs examined as described for NTP studies, 1990.
- Microscopic: Tissues examined as described for NTP studies, 1990. (Chhabra et al, NTP program, 1990)

STATISTICAL METHODS: ANOVA for body weight, food consumption, blood parameters and organ weights. Fischers Exact test for mortality, clinical observations and histopathological findings.

**Result** : NOAEL: >625 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 5, 25, 125, 625 mg/kg/day
- Time of death: No data
- Number of deaths at each dose: 1M control, 1M+1F at 5 mg/kg, 2M+1F at 625 mg/kg, confirmed by autopsy as due to the gavage procedure.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Clinical signs: Similar in treated and control animals.
- Body weight gain: Similar in treated and control animals.
- Food consumption: Similar in treated and control animals.
- Clinical chemistry: Similar in treated and control animals.
- Haematology: Similar in treated and control animals.
- Organ weights: Similar in treated and control animals.
- Gross pathology: Similar in treated and control animals.
- Histopathology: Similar in treated and control animals and in comparision with historical controls.

STATISTICAL RESULTS: No changes of statistical significance.

**Conclusion** : The NOAEL for this rat 90 day gavage study was >625 mg/kg/day. There were no treatment related changes in any of the parameters tested.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail.

**Flag** : Critical study for SIDS endpoint
16.05.2005 (7)

**Species** : rat

| | | |
|---|---|---|
| **Sex** | : | male/female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 1 year |
| **Frequency of treatment** | : | daily |
| **Post obs. period** | : | none |
| **Doses** | : | 0, 250, 500 and 1000 mg/kg |
| **Control group** | : | yes |
| **NOAEL** | : | > 1000 mg/kg bw |
| **Method** | : | other: |
| **Year** | : | 1998 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : C24-34 even chain alcohols (D-002) primarily isolated and purified from beeswax, composition as follows:

triacontanol 26.63%
octacosanol 17.49%
dotriacontanol 16.95%
hexacosanol 15.34%
tetracosanol 13.24%
tetratriacontanol % 2.23%
Other well-known, nonactive components 7.12%

**Test condition** : TEST ORGANISMS SD rats
- Age: 6-8 weeks
- Weight at study initiation: 150-200 g
- Number of animals: 20M+20F/group

ADMINISTRATION / EXPOSURE
- Duration of test/exposure: 1 year
- Type of exposure: gavage
- Post exposure period: none
- Vehicle: As a suspenson in acacia gum/water
- Concentration in vehicle: 10 mg/ml
- Doses: 0, 250, 500 and 1000 mg/kg

SATELLITE GROUPS AND REASONS THEY WERE ADDED: None

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: Daily
- Mortality: Daily
- Body weight: Weekly
- Food consumption: Weekly
- Water consumption: Not recorded
- Ophthalmoscopic examination: No data
- Haematology: Haemoglobin, Haematocrit, total and differential white cell count.
- Biochemistry: At the end of the assay. ALAT, ASAT, creatininte, acetyl cholinesterase, alkaline phosphatases, creatin-kinase, urea.
- Urinalysis: No

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopic: Organ weights are reported for liver, kidney, Heart, Lungs, Spleen and Thymus, organs examined as described for NTP studies, 1990.
- Microscopic: Tissues examined as described for NTP studies, 1990. (Chhabra et al, NTP program, 1990)

STATISTICAL METHODS: ANOVA for body weight, food consumption, blood parameters and organ weights. Fischers Exact test for mortality, clinical observations and histopathological findings.

**Result** : NOAEL: >1000 mg/kg/day

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX 5, 25, 125, 625 mg/kg/day
- Time of death: No data
- Number of deaths at each dose: 1M+1F control, 2M+1F at 250 mg/kg, 2M+2F at 500 and 1000 mg/kg, confirmed by autopsy as due to the gavage procedure.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Clinical signs: Similar in treated and control animals.
- Body weight gain: Similar in treated and control animals. However a slight non-significant decrease in bodyweight gain was observed at the top dose level.
- Food consumption: Similar in treated and control animals.
- Clinical chemistry: Similar in treated and control animals.
- Haematology: Similar in treated and control animals.
- Organ weights: Similar in treated and control animals.
- Gross pathology: Similar in treated and control animals.
- Histopathology: Similar in treated and control animals and in comparision with historical controls.

STATISTICAL RESULTS: No changes of statistical significance.

**Conclusion** : Rat gavage study NOAEL 1000 mg/kg/day for 1 year. A slight decrease in bodyweight gain in top dose animals was not of statistical significance. All other endpoints showed no adverse effect.

**Reliability** : (2) valid with restrictions
Study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not reported as being carried out to any specific regulatory guideline the conduct of the study appeared to similar to that required for a guideline study and the publication provided a good level of detail although not at the individual animal level.

**Flag** : Critical study for SIDS endpoint

16.05.2005 (7)

## 5.5 GENETIC TOXICITY ‘IN VITRO‘

## 5.6 GENETIC TOXICITY ‘IN VIVO‘

**Type** : Micronucleus assay
**Species** : mouse
**Sex** : male/female
**Strain** : NMRI
**Route of admin.** : gavage
**Exposure period** : 5 days
**Doses** : 2000 mg/kg/day
**Result** : negative
**Method** : other: similar to OECD 474
**Year** : 1998
**GLP** : no data

**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS: mouse NMRI
- Age: 40 days
- Weight at study initiation: 18-22 g
- No. of animals per dose: 6 male + 6 female

ADMINISTRATION: gavage
- Vehicle: suspension of gum arabic in water 10 mg gum arabic/kg
- Duration of test: 5 days
- Frequency of treatment: daily
- Sampling times and number of samples: Single sampling of bone marrow (ex femur) 24 hours after final dose.
_ Cells evaluated: 2000
- Control groups and treatment: vehicle control same treatment regime as the treated group, positive control cyclophosphamide single intraperitoneal dose of 50 mg/kg. Treated and vehicle controls received a constant dose volume of 1 ml/kg.

EXAMINATIONS:
- Clinical observations: Not reported
- Organs examined at necropsy: None
- Criteria for evaluating results: Total number of micronuclei, %PCE and PCE/NCE ratio.
- Criteria for selection of M.T.D.: Based on previous toxicity testing in this species the limit dose of 2000 mg/kg was used.

STATISTICAL ANALYSIS:
Increase in %PCE in total erythrocyte population evaluated using Mann Whitney U test, Comparision of PCE/NCE index between groups using Kruskall Wallis.

**Result** : MORTALITY: None

CLINICAL SIGNS: None reported

NECROPSY FINDINGS: None reported

BODY WEIGHT CHANGES: None reported

FOOD AND WATER CONSUMPTION CHANGES: Not reported

EFFECT ON PCE/NCE RATIO: No difference between treated and vehicle control groups significant reduction in positive controls.

PCE/NCE (determinations in 2000 erythrocytes/animal)
Vehicle control Male: 1.116 +- 0.23 Female: 1.18 +- 0.15
Treated 2000 mg/kg Male: 2.33 +- 0.25 Female: 1.09 +- 0.09
Positive control Male: 0.72 +- 0.15* Female: 0.73 +- 0.11*

* significant $p<0.05$ U (Mann Whitney)

GENOTOXIC EFFECTS: None

Total micronuclei (determinations in 2000 PCE/animal)
Vehicle control Male: 21 Female: 25
Treated 2000 mg/kg Male: 28 Female: 22
Positive control Male: 435 Female: 391

MN/PCE (determinations in 2000 PCE/animal) x 10 to power 3

Vehicle control Male: 1.75 +- 1.04 Female: 2.08 +- 0.66
Treated 2000 mg/kg Male: 2.33 +- 0.41 Female: 1.09 +- 0.09
Positive control Male: 37.73 +- 7.47* Female: 31.75 +- 8.08*

* significant p<0.05 U (Mann Whitney)

NOAEL (NOEL) (C) / LOAEL (LOEL) (C): NOAEL 2000 mg/kg/day

mPCE FREQUENCY: No significant difference between treated and control groups.

STATISTICAL RESULTS: See above

**Conclusion** : The product D-002 did not increase the numbers of micronucleated cells in the bone marrow of mice following repeated oral administration of the limit dose of 2000 mg/kg/day for 5 days.

**Reliability** : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not conducted specifically to OECD regulatory guidelines, the methodology appeared similar. Results were reported for the group (no individual animal results were provided in the publication)

**Flag** : Critical study for SIDS endpoint

12.04.2005 (6)

**Type** : Dominant lethal assay
**Species** : mouse
**Sex** : male/female
**Strain** : NMRI
**Route of admin.** : gavage
**Exposure period** : 6 weeks females; 8 weeks males
**Doses** : 0, 25, 125 and 625 mg/kg/day
**Result** : negative
**Method** : other: similar to OECD 478
**Year** : 1998
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Test condition** : TEST ORGANISMS: Mouse NMRI
- Age: 40 days
- Weight at study initiation: 18-20 g
- No. of animals per dose: 40 females/group; 25 males /group.

ADMINISTRATION: gavage
- Vehicle: suspension of gum arabic in water 10 mg gum arabic/kg
- Duration of test: 6 weeks for treated female groups, 8 weeks for males.
- Frequency of treatment: Daily
- Sampling times and number of samples:
- Control groups and treatment: vehicle control adminstered orally as for treated groups, 5 days intraperitoneally for positive control (cyclophosphamide 50 mg/kg) and control with saline.

EXAMINATIONS: At the end of the treatment period females were mated over a period of 1 week, 2 females to 1 untreated male. Treated males were mated with 2 females per male at two successive intervals each mating period being for one week to ensure that the effect of the drug was evaluated at 2 stages of spermatogenesis. The females from both studies were sacrificed 17-19 days after the first day of mating.
- Clinical observations: Mortality and body weight (recorded weekly)

- Organs examined at necropsy: uterus and ovaries
- Criteria for evaluating results: Number of implantations, late and early resorptions, % pregcant females, corpora lutea and numbers of live foetuses were examined.
- Criteria for selection of M.T.D.: A single oral dose produced no adverse effects at 5 g/kg/day. The study was designed to detect the cumulative effects of D-002.

STATISTICAL EVALUATION: Krusakall Wallis (non-parametric analysis of variance) for all parameters except frequency of mortality/pregnant female which used the Fischer Exact Probability test.

**Result** **:** MORTALITY: None

CLINICAL SIGNS: Not reported

NECROPSY FINDINGS: Not reported

BODY WEIGHT CHANGES: Not reported

FOOD AND WATER CONSUMPTION CHANGES: Not carried out

NOAEL: 625 mg/kg/day over a 6 week period for females or an 8 week period for males.

TEST PARAMETERS: Treated females n= 30-37
% Pregnant females/Implantations/Corpora lutea/Live foetuses/Early resorptions/Late resorptions per female/group
Vehicle control: 38/10.2/10.6/9.5/21 of 33/2 of 33
25 mg/kg 85/9.7/10.1/9.0/22 of 34/2 of 34
125 mg/kg 75/10.7/10.9/10.3/8 of 30/3 of 30
625 mg/kg 88/9.7/10.0/9.1/18 of 35/1 of 35
Saline control 91/11.1/12.3/10.5/15 of 36/5 of 36
Positive control 92/8.3*/12.2/4.7*/60 of 37**/52 of 37**

* p<0.05 Kruskall Wallis ** p<0.05 Fischer exact

Females (n =44-48) mated with treated males.
1st week of mating
% Pregnant females/Implantations/Corpora lutea/Live foetuses/Early resorptions/Late resorptions per female/group
Vehicle control: 92/12.8/13.8/12.1/ 25 of 46/ 5 of 46
25 mg/kg: 88/11.4/12.8/10.7/ 32 of 44/ 2 of 44
125 mg/kg: 94/11.8/13.4/11.1/ 31 of 47/ 2 of 47
625 mg/kg: 94/12.0/13.1/11.5/ 19 of 47/ 2 of 47
saline control: 95/11.1/12.5/10.3/ 23 of 48/ 2 of 48
positive control: 83/7.7*/11.3/4.2*/ 87 of 46**/ 62 of 46**

* p<0.05 Kruskall Wallis ** p<0.05 Fischer exact

Results for the second week of mating followed a similar pattern to those reported above.

STATISTICAL RESULTS: See above

**Conclusion** **:** There is no evidence of dominant lethality in the mouse following repeated oral exposure to D-002 at dose levels up to 625 mg/kg/day for 6 weeks in females and 8 weeks in males as indicated by early and late resorptions, foetal survival, numbers of corpora lutea and numbers of implantations/female/group.

| | | |
|---|---|---|
| **Reliability** | : | (2) valid with restrictions<br>Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment. Although not conducted specifically to OECD regulatory guidelines, the methodology appeared similar. Results were reported for the group (no individual animal results were provided in the publication) |
| **Flag** | : | Critical study for SIDS endpoint |

12.04.2005 (6)

## 5.7 CARCINOGENITY

## 5.8.1 TOXICITY TO FERTILITY

| | | |
|---|---|---|
| **Type** | : | other: Repeat dose study with histopathology of reproductive organs. |
| **Species** | : | dog |
| **Sex** | : | male/female |
| **Strain** | : | Beagle |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | 1 year |
| **Frequency of treatment** | : | daily |
| **Premating exposure period** | | |
| **Male** | : | |
| **Female** | : | |
| **Duration of test** | : | 1 year |
| **Doses** | : | 50, 250 mg/kg bw |
| **Control group** | : | yes |
| **NOAEL Parental** | : | = 250 mg/kg bw |
| **Method** | : | other |
| **Year** | : | 2001 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Test substance** | : | A C24-C34 alcohol, called D-002, primarily isolated and purified from beeswax. The composition is C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% of "other well known, non-active substances". C24-34 even alcohol (D-002) |
| **Test condition** | : | Groups of 4M + 4F dogs received 0, 50 or 250 mg/kg/day by gavage for a year. Full details of this study are to be found in Chapter 5.4: Repeated dose toxicity. Weights of the testes and prostate gland were measured and the testes, prostate, penis, ovaries, uterus and vagina were examined histopathologically. |
| **Result** | : | No deaths occurred during the study. There were no clinical symptoms of toxicity observed and no significant difference in body weight gain between controls and test animals. Testes weight in treated groups was comparable to that of the controls. Ovaries were not weighed. Histopathological examination of the reproductive organs in both sexes revealed no treatment related changes. The NOAEL for effects on the reproductive organs is 250 mg/kg/day |
| **Reliability** | : | (2) valid with restrictions<br>Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment. |

**Source** : Aleman 2001.
Hayes Consultancy Service Bromley, Kent

24.01.2005 (1)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

| | | |
|---|---|---|
| **Species** | : | rat |
| **Sex** | : | female |
| **Strain** | : | Sprague-Dawley |
| **Route of admin.** | : | gavage |
| **Exposure period** | : | gestation days 6-15 |
| **Frequency of treatment** | : | daily |
| **Duration of test** | : | day 20 |
| **Doses** | : | 100, 320, 1000 mg/kg bw |
| **Control group** | : | yes, concurrent vehicle |
| **NOAEL Maternalt.** | : | = 1000 mg/kg bw |
| **NOAEL Teratogen** | : | = 1000 mg/kg bw |
| **Method** | : | other: see text |
| **Year** | : | 1998 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : A C24-C34 alcohol, called D-002, the components of which are primarily isolated and purified from beeswax. The composition was C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% "other well known, non-active substances". C24-34 even alcohols (D-002)

**Test condition** : TEST ORGANISMS Groups of 25 presumed pregnant females weight 175-204 g.

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage on gestation days 6-15
- Duration of test/exposure: 20 days
- Treatment: 0, 100, 320 and 1000 mg/kg/day
- Control group and treatment: Concurrent, 10 mg/ml gum acacia suspension.
- Vehicle: 10 mg/ml gum acacia
- Concentration in vehicle: Variable to give a constant dosing volume.
- Total volume applied: 2 ml/kg

MATING PROCEDURES: 2 females to 1 male

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Not reported.
- Clinical observations: Daily
- Examination of uterine content: Day 20, numbers of implants, resorptions and dead foetuses were recorded. The ovaries were examined for numbers of corpora lutea. Uteri of apparently non-pregnant animals were examined for evidence of implantation.
- Examination of fetuses: All live foetuses were examined externally and half were examined viscerally the other half for skeletal anomalies.

STATISTICAL METHODS: Maternal and foetal weights analyses by parametric analysis of variance followed by the Tukey test. Reproductive parameters were examined by the Kruskall-Wallis test. The incidence of malformations and skeletal variations was carried out using the Fischer exact test.

**Result** : NOAEL: 1000 mg/kg/day for maternal toxicity, foetotoxicity and teratogenicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 320 and 1000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 21 controls, 19 at 100 mg/kg/day, 22 at 320 and 1000 mg/kg/day
- Number aborting: None
- Number of resorptions, implantations, pre and post implantation loss: Comparable in treated and control groups. No Implantation sites mean 10.1, 9.2, 10.8 and 10.1; % resorptions (early) 4, 1, 2 and 4 for controls, low, mid and high dose respectively.
- Number of corpora lutea: Comparable in treated and control groups. Mean corpora lutea 11.6, 11.8, 12.4 and 11.5 for controls, low, mid and high dose respectively.
- Body weight: No statistical differences between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None observed.

FOETAL DATA:
- Litter size and weights, number viable, sex ratio: No statistically significant differences between treated and control groups. Number of live foetuses mean 9.9, 8.9, 10.7 and 9.9; mean foetal weight 3.8, 4.0, 3.8 and 4.1 gm; Sex ratio male/female 1.22, 0.8, 1.26 and 1.13 for controls, low, mid and high dose respectively.
- External abnormalities: A single foetus with exencaphaly in the controls none in the treated group.
- Soft tissue abnormalities: None
- Skeletal abnormalities: Foetuses with supernumary or rudimentary ribs and retarded, rudimentary or asymmetrical ossification of the sternal centrum were observed in all treated and control groups the incidence was comparable between treated and control groups and without statistical significance. Incidence of foetuses with variations 10, 8, 13 and 6% for controls, low, mid and high dose groups respectively.

**Conclusion** : The NOAEL for maternal toxicity, teratogenicity and foetotoxicity in rats receiving C24-34 alcohol on gestation days 6-15 is 1000 mg/kg, the highest dose level tested. This is based on a lack of adverse effects in any of the parameters of maternal, reproductive or foetal toxicity investigated.

**Reliability** : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Rodriguez, 1998
Hayes Consultancy Service Bromley, Kent

**Flag** : Critical study for SIDS endpoint
24.01.2005 (8)

**Species** : rabbit
**Sex** : female
**Strain** : New Zealand white
**Route of admin.** : gavage
**Exposure period** : day 6-18 of gestation
**Frequency of treatment** : daily

| | | |
|---|---|---|
| **Duration of test** | : | 29 days |
| **Doses** | : | 100, 320 and 1000 mg/kg bw |
| **Control group** | : | yes, concurrent vehicle |
| **NOAEL Maternalt.** | : | > 1000 mg/kg bw |
| **NOAEL Teratogen** | : | > 1000 mg/kg bw |
| **Method** | : | other: see text |
| **Year** | : | 1998 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Test substance** : A C24-C34 alcohol, called D-002, primarily isolated and purified from beeswax. The composition is C24 (13.2%), C26 (15.3%), C28 (17.5%), C30 (26.6%), C32 (17%), C34 (2.2%) and 7% of "other well known, non-active substances". C24-34 even alcohol (D-002)

**Test condition** : TEST ORGANISMS Groups of 16-20 presumed pregnant females weight 2.5-3.5 kg.

ADMINISTRATION / EXPOSURE
- Type of exposure: gavage on gestation days 6-15
- Duration of test/exposure: 29 days
- Treatment: 0.100, 320 and 1000 mg/kg/day
- Control group and treatment: Concurrent, 10 mg/ml gum acacia suspension.
- Vehicle: 10 mg/ml gum acacia
- Concentration in vehicle: Variable to give a constant dosing volume.
- Total volume applied: 2 ml/kg

MATING PROCEDURES: Mated with males of the same breed until copulation was opbserved

PARAMETERS ASSESSED DURING STUDY:
- Body weight gain: Daily
- Food consumption: Not reported.
- Clinical observations: Daily
- Examination of uterine content: Day 20, numbers of implants, resorptions and dead foetuses were recorded. The ovaries were examined for numbers of corpora lutea. Uteri of apparently non-pregnant animals were examined for evidence of implantation.
- Examination of fetuses: All live foetuses were examined externally and for visceral and skeletal anomalies.

STATISTICAL METHODS: Maternal and foetal weights analyses by parametric analysis of variance followed by the Tukey test. Reproductive parameters were examined by the Kruskall-Wallis test. The incidence of malformations and skeletal variations was carried out using the Fischer exact test.

**Result** : NOAEL: 1000 mg/kg/day for maternal toxicity, teratogenicity and foetotoxicity.

ACTUAL DOSE RECEIVED BY DOSE LEVEL BY SEX: 0, 100, 320 adn 1000 mg/kg/day

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:
- Mortality and day of death: None
- Number pregnant per dose level: 20 controls, 16 at 1000 mg/kg/day, 17 at 320 mg/kg/day, 19 at 1000 mg/kg/day
- Number aborting: None
- Number of resorptions & implantations, pre and post implantation loss,

number of corpora lutea: Comparable in treated and control groups. Corpora lutea (mean) 7.6, 6.8, 7.4 and 7.1; Implantation sites (mean) 6.7; 5.9, 6.4 and 5.6; Resorptions 4, 2, 2 and 6%; Early resorptions 5, 0, 4 and 4%; Late resorptions 0, 4, 0 and 3% for controls, low, mid and high dose respectively.
- Duration of Pregnancy: Comparable in treated and control groups.
- Body weight: No statistically significant differences between treated and control groups.
- Description, severity, time of onset and duration of clinical signs: None observed.

FETAL DATA:
- Litter size and weights, viability, sex ratio: no differences between treated and control groups. No of live foetuses (mean) 6.3, 5.8, 6.1 and 5.1; Mean foetal weight 29.3, 30.7, 32.8 and 33.7 gm; Sex ration male/female 1.05, 1.12, 1.42 and 1.58 for controls, low, mid and high dose respectively.
- External abnormalities: 1 control foetus with acephaly, At 320 mg/kg/day two foetuses from different litters had hemivertebra with fused thoracic ribs.
- Soft tissue abnormalities: None
- Skeletal abnormalities: All groups showed skeletal variation such as extra rib or a pair of ribs, retarded ossification of the sternum, cleaved and fused sternal centra. The incidence of these variations was not dose related. Incidence of foetuses with variations 50, 48, 41 and 51% for controls, low, mid and high dose respectively.

**Conclusion** : The NOAEL for maternal toxicity, teratogenicity and foetotoxicity is 1000 mg/kg, the highest dose level tested. This is based on a lack of adverse effects in any of the parameters of maternal, reproductive or foetal toxicity investigated.

**Reliability** : (2) valid with restrictions
Publication, study well documented, meets generally accepted scientific principles, acceptable for assessment.

**Source** : Rodriguez, 1998
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**Flag** : Critical study for SIDS endpoint

24.01.2005 (8)

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

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(8) Rodriguez, MD, R Gamez, M Sanchez and H Garcia. 1998. Developmental Toxicity of D-002 (a Mixture of Aliphatic Primary Alcohols) in Rats and Rabbits. Journal of Applied Toxicology, 18, 313-316.