

201-158965

**UNITED STATES  
ENVIRONMENTAL PROTECTION AGENCY (EPA)  
HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

**ROBUST SUMMARIES DOSSIER  
for MEMBERS of the  
HIGHER OLEFINS CATEGORY  
CONTAINING C14 - C16 OLEFINS**

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**Members containing C14-C16 olefins:**

CAS No. 629-73-2, 1-Hexadecene  
CAS No. 68855-58-3, Alkenes, C10-16 alpha  
CAS No. 68855-59-4, Alkenes, C14-18 alpha  
CAS No. 68855-60-7, Alkenes, C14-20 alpha  
CAS No. 68991-52-6, Alkenes, C10-16  
CAS No. 93762-80-2, Alkenes, C15-18  
CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Contains Robust Summaries for the Following Substances:**

CAS No. 1120-36-1, 1-Tetradecene  
CAS No. 26952-13-6, Tetradecene  
CAS No. 27251-68-9, Pentadecene  
CAS No. 629-73-2, 1-Hexadecene  
CAS No. 26952-14-7, Hexadecene  
C12-16 Alpha Olefin Fraction (GULFTENE 12-16)  
CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons  
CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%)  
CAS No. 68855-59-4, C14-16 Alpha Olefin Blend

**Prepared by:**

**American Chemistry Council  
Higher Olefins Panel**

**April 28, 2005**

## 1. GENERAL INFORMATION

### 1.01 Details on Chemical Category

The Higher Olefins Category consists of a non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins (C<sub>6</sub> through C<sub>54</sub>) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The C<sub>6</sub> – C<sub>14</sub> even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the C<sub>6</sub>, C<sub>7</sub>, C<sub>8</sub>, C<sub>9</sub>, C<sub>10</sub>, C<sub>12</sub> and C<sub>10-13</sub> aliphatic linear and branched internal olefins and the C<sub>16</sub> and C<sub>18</sub> aliphatic linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). The members of the category are presented below.

### Members of the Higher Olefins Category

Alpha Olefins	Branched/Linear	CAS No.
Neohexene	Branched	558-37-2
1-Tridecene	Linear	2437-56-1
1-Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-9
1-Eicosene	Linear	3452-07-1
1-Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
<b>Internal Olefins</b>		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	Branched and Linear	68526-53-4
Alkenes, C7-9, C8-rich	Branched and Linear	68526-54-5
Alkenes, C8-10, C9-rich	Branched and Linear	68526-55-6
Alkenes, C9-11, C10-rich	Branched and Linear	68526-56-7
Alkenes, C10-12, C11-rich	Branched and Linear	68526-57-8
Alkenes, C11-13, C12-rich	Branched and Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9

C12,14 Olefin rich hydrocarbons	Linear	68514-33-0
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## 1.1 General Substance Information

### A. Type of Substance

Element [ ]; Inorganic [ ]; Natural substance [ ]; Organic [X]; Organometallic [ ];  
Petroleum product [ ]

### B. Physical State (at 20°C and 1.013 hPa)

Gaseous [ ]; Liquid [X]; Solid [ ]

**C. Purity:** C14, C15 and/or C16 containing category members are manufactured and marketed as blends. 1-Hexadecene is also manufactured and marketed as a pure product. The purity of 1-hexadecene has been reported as 92% and as 80-98%.

## 1.2 Impurities

**Remark:** The compositions reported by manufacturers for the members of the Higher Olefins Category containing C14-C16 olefins are shown below:

Alpha Olefins	CAS No.	Composition/Impurities
1-Hexadecene	629-73-2	5.5-6.8% vinylidenes (branching at 2 <sup>nd</sup> carbon), max. 7% C14 and lower olefins, max. 15% C18 and higher olefins
Alkenes, C10-16 alpha	68855-58-3	Typical composition: 0.6% C10, 64.2% C12, 34.7% C14, 0.5% C16; 99.6% monoolefin; 0.4% paraffin; 86.5% linear terminal; 10.6% branched terminal; 2.9% linear internal
Alkenes, C14-18 alpha	68855-59-4	Typical composition: 1% C12, 65% C14, 33% C16, 1% C18; 99.5% monoolefin; 0.5% paraffin; 82.0% linear terminal; 14% branched terminal; 4% linear internal
Alkenes, C14-20 alpha	68855-60-7	Typical composition: 1% C14, 57% C16, 37% C18, 5% C20; 99.2% monoolefin; 0.8% paraffin; 61.5% linear terminal; 32.5% branched terminal; 6% linear internal
<b>Internal Olefins</b>		
Alkenes, C10-16	68991-52-6	Mostly linear, less than 2% branched.
Alkenes, C15-C18	93762-80-2	Mostly linear, less than 2% branched.
C12,14 Olefin rich hydrocarbons	68514-33-0	0-8% C12 and lower, 92-100% C14, 0-0.2% C16, 0-1% C14, 0-50% paraffins

### 1.3 Additives

None

### 1.4 Synonyms

### 1.5 Quantity

Remarks:

U.S. production volumes for C14, C15 and C16 containing members of the Higher Olefins Category reported for 2002 by members of the American Chemistry Council's Higher Olefins Panel:

COMPOUND	CAS NUMBER	2002 PRODUCTION VOLUME (Million Pounds)
<b>Alpha Olefins</b>		
1-Hexadecene	629-73-2	100-200
Alkenes, C10-16 alpha	68855-58-3	1-10
Alkenes, C14-18 alpha	68855-59-4	1-10
Alkenes, C14-20 alpha	68855-60-7	50-100
<b>Internal Olefins</b>		
Alkenes, C10-16	68991-52-6	400-500
Alkenes, C15-C18	93762-80-2	700-800
C12,14 Olefin rich hydrocarbons	68514-33-0	1-10

Reference:

American Chemistry Council's Higher Olefins Panel (2002)

### 1.6 Use Pattern

**Type of Use:**

(a) Main  
Industrial  
Use

Remarks:

**Category:**

Use in closed systems  
Chemical industry – chemicals used in synthesis  
Intermediate

Intermediate in the manufacture of lube oil additives, hydraulic fluids and additives, surfactants, detergent alcohols and nonionics; and may be blended with other chemicals for use as drilling fluids for off-shore oil exploration

(b) Main

Non-dispersive use



**C. Options for Disposal**

Remarks: Incineration or diversion to other hydrocarbon uses

**D. Last Literature Search**

**Type of search:** Internal and external  
**Date of search:** October 2003  
**Remark:** Medline  
IUCLID  
TSCATS  
ChemIDplus  
AQUIRE - ECOTOX

**2. PHYSICAL CHEMICAL DATA**

**2.1 Melting Point**

**A. Test Substance**

Identity: CAS No. 629-73-2, 1-Hexadecene or CAS No. 26952-14-7, Hexadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN v. 3.11,  
subroutine MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula  $T_m = 0.5839T_b$ , where  $T_m$  is the melting point in Kelvin and  $T_b$  is the boiling point in Kelvin. EPIWIN used the alpha structure for 1-hexadecene and the structure for 2-hexadecene for the internal olefin.

**Results**

Melting point  
value in °C: 21°C

**Flag:** Key study for SIDS endpoint

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**References:** Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method/  
guideline followed:** Not reported  
**GLP:** Not reported  
**Year:**

**Test Conditions:** Not reported

**Results**

**Melting point  
value in °C:** 4.1°C

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

**C. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

**Method/  
guideline followed:** Calculated value using the computer program EPIWIN v. 3.11, subroutine MPBPWIN v 1.41  
**GLP:** Not applicable  
**Year:** Not applicable

**Test Conditions:** Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982).

The Gold and Ogle Method simply uses the formula  $T_m = 0.5839T_b$ , where  $T_m$  is the melting point in Kelvin and  $T_b$  is the boiling point in Kelvin. Program used the structure for 2-pentadecene.

### Results

Melting point  
value in °C:

11.04°C

**Reliability:**

(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**Flag:**

Key study for SIDS endpoint

**References:**

Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### D. Test Substance

Identity:

CAS No. 1120-36-1, 1-Tetradecene

### Method

Method/  
guideline followed:  
GLP:  
Year:

Not reported  
Not reported

**Test Conditions:**

Not reported

### Results

Melting point  
value in °C:

-12°C

**Reliability:**

(2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**Flag:**

Key study for SIDS endpoint

**References:**

Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

### E. Test Substance

**Identity:** CAS No.26952-13-6, Tetradecene

**Method**

**Method/  
guideline followed:** Calculated value using the computer program EPIWIN v. 3.11,  
subroutine MPBPWIN v 1.41

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula  $T_m = 0.5839T_b$ , where  $T_m$  is the melting point in Kelvin and  $T_b$  is the boiling point in Kelvin. Program used the structure for 2-tetradecene.

**Results**

**Melting point  
value in °C:** 0.41°C

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**Flag:** Key study for SIDS endpoint

**References:** Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

**Identity:** CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Method/  
guideline followed:** Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982).

The Gold and Ogle Method simply uses the formula  $T_m = 0.5839T_b$ , where  $T_m$  is the melting point in Kelvin and  $T_b$  is the boiling point in Kelvin. Program used a C12 structure with double bonds in 4 locations.

## Results

Melting point  
value in °C:

-24.15°C

**Reliability:**

(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

**Flag:**

Key study for SIDS endpoint

**References:**

Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## 2.2 Boiling Point

### A. Test Substance

Identity:

CAS No. 629-73-2, 1-Hexadecene

### Method

Method/  
guideline followed:

Calculated value using the computer program EPIWIN MPBPWIN v 1.41

GLP:

Not applicable

Year:

Not applicable

**Test Conditions:**

Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994).

## Results

Boiling point  
value in °C:

275.88°C

Pressure:

1013

Pressure unit:

hPa

**Reliability:**

(2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method/  
guideline followed:** Not reported  
**GLP:** Not reported  
**Year:** Not reported

**Test Conditions:**

**Results**

**Boiling point  
value in °C:** 284.9°C  
**Pressure:** 1013  
**Pressure unit:** hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

**C. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method/  
guideline followed:** Not reported  
**GLP:** Not reported  
**Year:** Not reported

**Test Conditions:**

**Results**

Boiling point  
value in °C: 272-274 °C  
Pressure: 1013  
Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**References:** Shell Product Brochure for Neodene: Alpha and Internal Olefins, SC 1095-94R, Shell Chemicals Europe Ltd.

**D. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 2-pentadecene.

**Results**

Boiling point  
value in °C: 265.77°C  
Pressure: 1013  
Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

Identity: CAS No. 26952-14-7, Hexadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN MPBPWIN v  
1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 2-hexadecene.

**Results**

Boiling point  
value in °C: 281.97°C

Pressure: 1013

Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

Identity: CAS No. 1120-36-1, 1-Tetradecene

**Method**

Method/  
guideline followed: Not reported

GLP: Not reported

Year: Not reported

**Test Conditions:**

**Results**

Boiling point

value in °C: 252.1°C  
Pressure: 1013  
Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Weiss G. (1986). Hazardous Chemical Data Book, Noyes Data Corporation, Park Ridge, NJ, 2<sup>nd</sup> edition

### G. Test Substance

Identity: CAS No.26952-13-6, Tetradecene

#### Method

Method/  
guideline followed: Calculated value using the computer program EPIWIN MPBPWIN v  
1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 2-tetradecene.

#### Results

Boiling point  
value in °C: 248.65°C  
Pressure: 1013  
Pressure unit: hPa

**Reliability:** (2) Reliable with restrictions. The result includes calculated data based on chemical structure as modeled by EPIWIN

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### H. Test Substance

**Identity:** CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Method**

**Method/  
guideline followed:** Calculated value using MPBPWIN version 1.41, a subroutine of  
EPIWIN version 3.11

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used a C12 structure with double bonds in 4 locations.

**Results**

**Boiling point  
value in °C:** 229.23°C

**Pressure:** 1013

**Pressure unit:** hPa

**Reliability:** (2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.  
EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**2.3 Density (Relative Density)**

**A. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Remarks:** Purity approx. 92%

**Method**

**Method:** ASTM D 287

**GLP:** No

**Test Conditions:** No data

**Results**

**Type:** Relative Density  
**Value:** 0.7853  
**Temperature (°C):** 15.6/15.6  
**Reliability:** (1) Reliable without restrictions.  
**Reference:** Chevron Phillips Chemical Company, The Woodlands, TX (unpublished report)

**B. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method:** No data  
**GLP:** No

**Test Conditions:** No data

**Results**

**Type:** Relative Density

**Value:** 0.7811

**Temperature (°C):** 20 °C

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.

**Reference:** Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

**C. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method:** No data  
**GLP:** No

**Test Conditions:** No data

**Results**

Type: Density  
Value: 0.7745  
Temperature (°C): 20 °C  
**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not reviewed for quality.  
**Reference:** Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

## 2.4 Vapour Pressure

### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

#### Method

Method/  
guideline followed: Not reported  
GLP: Not applicable  
Year:

#### Test Conditions:

#### Results

Vapor Pressure  
value: 0.00352 hPa  
Temperature: 25°C  
Remarks: Reported as 0.00264 mm Hg (25°C)

**Reliability:** (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Daubert, T.E. and R.P. Danner (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY; EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### B. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

**Method**

Method/  
guideline followed: Not reported  
GLP: No data  
Year:

**Test Conditions:** No data

**Results**

Vapor Pressure  
value: <0.069 hPa  
Temperature (°C): 37.8°C

**Reliability:** (2) Reliable with restrictions. Reliable source but data were not reviewed for quality.

**References:** Shell Product Brochure for Neodene: Alpha and Internal Olefins, SC 1095-94R, Shell Chemicals Europe Ltd.

**C. Test Substance**

Identity: CAS No. 629-73-2, 1-Hexadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. Used experimental value for BP of 284.90 °C from EPIWIN database

**Results**

Vapor Pressure  
value: 0.0102 hPa  
Temperature (°C): 25°C  
Remarks: Reported as 0.00766 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN using measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**References:** Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

**Method**

**Method/  
guideline followed:** Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the modified Grain Method described by Neely and Blau, 1985. Used value for BP of 281.97 °C (estimated by EPIWIN using the structure for 2-hexadecene).

**Results**

**Vapor Pressure  
value:** 0.0118 hPa  
**Temperature (°C):** 25°C  
**Remarks:** Reported as 0.00887 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN using data estimated by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

Method/  
guideline followed: Not reported  
GLP: Not applicable  
Year:

**Test Conditions:**

**Results**

Vapor Pressure  
value: 0.0120 hPa  
Temperature: 25°C  
Remarks: Reported as 0.015 mm Hg (25°C)

**Reliability:** (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

**Flag:** Key study for SIDS endpoint

**References:** Daubert, T.E. and R.P. Danner (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY; EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

Identity: CAS No.26952-13-6, Tetradecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. Used value for BP of 248.65 °C (estimated by EPIWIN using the structure for 2-tetradecene).

**Results**

Vapor Pressure  
value: 0.0631 hPa

Temperature (°C): 25°C  
Remarks: Reported as 0.0473 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN using data estimated by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals. Volume 1, p. 31, CRC Press.

**G. Test Substance**

Identity: CAS No. 27251-68-9, Pentadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN, MPBPWIN v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. Used value for BP of 265.77 °C estimated using EPIWIN with a structure for 2-pentadecene.

**Results**

Vapor Pressure  
value: 0.0261 hPa

Temperature (°C): 25°C

Remarks: Reported as 0.0196 mm Hg

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN using data estimated by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## H. Test Substance

**Identity:** CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

### Method

**Method/  
guideline followed:** Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11

**GLP:** Not applicable

**Year:**

**Test Conditions:** Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used a value for BP of 229.23 °C estimated by EPIWIN using a C12 structure with double bonds in 4 locations.

### Results

**Vapor Pressure  
Value:** 0.1667 hPa  
**Temperature:** 25°C  
**Remarks:** Reported as 0.125 mm Hg (25°C)

**Reliability:** (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

**Flag:** Key study for SIDS endpoint

**References:** Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## 2.5 Partition Coefficient (log<sub>10</sub>K<sub>ow</sub>)

### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

#### Method

Method: Calculated value using the computer program EPIWIN, KOWWIN v  
1.67

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995).

#### Results

Log K<sub>ow</sub>: 8.0626

Temperature (°C): Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### B. Test Substance

Identity: CAS No. 26952-14-7, Hexadecene

#### Method

Method: Calculated value using the computer program EPIWIN, KOWWIN v  
1.67

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 2-hexadecene.

**Results**

Log Kow: 7.98  
Temperature (°C): Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Test Substance**

Identity: CAS No. 27251-68-9, Pentadecene

**Method**

Method: Calculated value using the computer program EPIWIN, KOWWIN v 1.67  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 2-pentadecene.

**Results**

Log Kow: 7.49  
Temperature (°C): Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method:** Calculated value using the computer program EPIWIN, KOWWIN v 1.67  
**GLP:** Not applicable  
**Year:** Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995).

**Results**

**Log Kow:** 7.08  
**Temperature (°C):** Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

**E. Test Substance**

Identity: CAS No.26952-13-6, Tetradecene

**Method**

Method: Calculated value using the computer program EPIWIN, KOWWIN v 1.67

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 2-tetradecene.

**Results**

Log Kow: 7.00

Temperature (°C): Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

Identity: CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Method**

Method: Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of

Meylan and Howard (1995). Program used a C12 structure with double bonds in 4 locations.

**Results**

Log Kow: 5.37  
Temperature (°C): Not applicable

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

**Flag:** Key study for SIDS endpoint

**Reference:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**2.6.1 Water Solubility (including \*Dissociation Constant).**

**A. Test Substance**

Identity: CAS No. 629-73-2, 1-Hexadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN,  
WSKOW v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 8.06 (estimated by EPIWIN).

**Results**

Value(mg/L) at  
temperature ( °C): 0.00144 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated.

**Flag:** Key study for SIDS endpoint

**References:** Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method/  
guideline followed:** Calculated value using the computer program EPIWIN, WATERNT v 1.01

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** The water solubility is calculated by the WATERNT subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995).

**Results**

**Value(mg/L) at  
temperature ( °C):** 0.00039982 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EPIWIN.

**References:** Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN,  
WSKOW v 1.41  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 7.98 (estimated by EPIWIN using the structure for 2-hexadecene).

### Results

Value(mg/L) at  
temperature ( °C): 0.00144 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated.

**Flag:** Key study for SIDS endpoint

**References:** Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### D. Test Substance

Identity: CAS No. 27251-68-9, Pentadecene

#### Method

Method/  
guideline followed: Calculated value using the computer program EPIWIN,  
WSKOW v 1.41  
GLP: Not applicable  
Year: Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 7.49 (estimated by EPIWIN using the structure for 2-pentadecene).

### Results

Value(mg/L) at  
temperature ( °C): 0.00448 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated.

**Flag:** Key study for SIDS endpoint

**References:** Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method/  
guideline followed:** Calculated value using the computer program EPIWIN,  
WSKOW v 1.41

**GLP:** Not applicable

**Year:** Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 7.08 (estimated by EPIWIN) and a melting point of -12°C .

**Results**

**Value(mg/L) at  
temperature ( °C):** 0.01353 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated.

**Flag:** Key study for SIDS endpoint

**References:** Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

**Identity:** CAS No.26952-13-6, Tetradecene

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN,  
WSKOW v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 7.00 (estimated by EPIWIN using the structure for 2-tetradecene).

**Results**

Value(mg/L) at  
temperature ( °C): 0.0139 mg/L (25°C)

**Reliability:** (2) Reliable with restrictions. The result was calculated.

**Flag:** Key study for SIDS endpoint

**References:** Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**G. Test Substance**

**Identity:** CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Method**

Method/  
guideline followed: Calculated value using the computer program EPIWIN 3.11,  
subroutine WSKOW v 1.41

GLP: Not applicable

Year: Not applicable

**Test Conditions:** Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 5.37 used for

calculation. EPIWIN used a C12 structure with double bonds in 4 locations to calculate Log Kow.

## Results

Value(mg/L) at  
temperature ( °C):

0.4989 mg/L (25°C)

**Reliability:**

(2) Reliable with restrictions. The result is a calculated value.

**Flag:**

Key study for SIDS endpoint

**References:**

Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## 2.6.2 Surface tension

No data available

## 2.7 Flash Point (Liquids)

### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

### Method

Method: No data

GLP: No data

**Test Conditions:** No data

### Results

Value (°C): 126.7 °C

Type of test: closed cup

**Reliability:**

(2) Reliable with restrictions. Reliable secondary source but data were not evaluated for quality.

**Reference:**

Shell Product Brochure for Neodene: Alpha and Internal Olefins, SC 1095-94R, Shell Chemicals Europe Ltd.

**B. Test Substance**

Identity: CAS No. 629-73-2, 1-Hexadecene  
Remarks: Purity approx. 92%

**Method**

Method: ASTM D93  
GLP: No data

**Test Conditions:** No data

**Results**

Value (°C): 132 °C  
Type of test: Pensky-Martens closed cup tester

**Reliability:** (2) Reliable with restrictions. Test conducted by reliable testing facility but data were not evaluated for quality.

**Reference:** Chevron Phillips Chemical Company Product Brochure, Company test results, Chevron Phillips Chemical Company, The Woodlands, TX.

**C. Test Substance**

Identity: CAS No. 1120-36-1, 1-Tetradecene

**Method**

Method: No data  
GLP: No data

**Test Conditions:** No data

**Results**

Value (°C): 107.2 °C  
Type of test: closed cup

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data were not evaluated for quality.

**Reference:** Lappin, G.R. and J.D. Sauer (1989) Alpha Olefins Application Handbook, Marcel Dekker, Inc., N.Y.

## 2.8 Auto Flammability (Solids/Gases)

### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene  
Remarks: Purity approx. 92%

#### Method

Method: No data  
GLP: No

**Test Conditions:** No data

#### Results

Value (°C): 224 °C  
Pressure (hPa): No data

**Reliability:** (2) Reliable with restrictions. Test conducted by reliable testing facility but data were not evaluated for quality.

**Reference:** Chevron Phillips Chemical Company Product Brochure, Company test results, Chevron Phillips Chemical Company, The Woodlands, TX.

### B. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

#### Method

Method: No data  
GLP: No

**Test Conditions:** No data

#### Results

Value (°C): 240 °C  
Pressure (hPa): 1013.25 hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data was not evaluated for quality.

**Reference:** Hilado, C.J. and S.W. Clark (1972) Autoignition temperatures of organic chemicals. Chemical Engineering. September 4, p.76.

### C. Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method:** No data

**GLP:** No

**Test Conditions:** No data

**Results**

**Value (°C):** 239 °C

**Pressure (hPa):** 1013.25 hPa

**Reliability:** (2) Reliable with restrictions. Reliable secondary source. Data was not evaluated for quality.

**Reference:** Hilado, C.J. and S.W. Clark (1972) Autoignition temperatures of organic chemicals. Chemical Engineering. September 4, p.76.

**2.9 Flammability**

**Result:** Non flammable

**Method:** Defined by flash point

**2.10 Explosive Properties**

**Result:** Not explosive

**Method:** Based on thermodynamic information

**2.11 Oxidising Properties**

**Result:** No oxidizing properties

**Method:** Based on structural formula

**2.12 Oxidation-Reduction Potential**

Not applicable

**3. ENVIRONMENTAL FATE AND PATHWAYS**

**3.1 Stability**

**A. Photodegradation**

**(1) Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene; CAS No. 26952-14-7, Hexadecene; CAS No. 27251-68-9, Pentadecene; CAS No. 1120-36-1, 1-Tetradecene; or CAS No. 26952-13-6, Tetradecene

**Method**

**Method/  
guideline followed:** Other: Technical discussion

**Type:** water  
**GLP:** Not applicable  
**Year:** Not applicable

**Test Conditions:** Not applicable

**Results**

**Direct photolysis:** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Higher Olefins Category.

**Remarks:** The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in

proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Olefins with one double bond, such as the chemicals in the Higher Olefins category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerization about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (Harris, 1982a).

Products in the Higher Olefins Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

**Reliability:** Not applicable

**References:** Harris J C (1982a). Rate of Aqueous Photolysis. Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline (1977). Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

(2) **Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method/  
guideline followed:** Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.10 which uses a program described by Meylan, W.M. and Howard, P.H. (1993)

**Type:** air  
**GLP:** Not applicable  
**Year:** Not applicable

**Results**

Indirect photolysis

**Sensitiser (type):** OH  
**Rate Constant:** 44.3085 E-12 cm<sup>3</sup>/molecule-sec  
**Degradation % after:** 50% after 2.897 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>)

**Sensitiser (type):** Ozone

Rate Constant: 1.2 E-17 cm<sup>3</sup>/molecule-sec  
Degradation % after: 50% after 22.920 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

**Reliability:** (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

**Flag:** Critical study for SIDS endpoint

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 26: 2293-99.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### (3) Test Substance

**Identity:** CAS No. 26952-14-7, Hexadecene

#### Method

**Method/  
guideline followed:** Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.10 which uses a program described by Meylan, W.M. and Howard, P.H. (1993). Program used the structure for 2-hexadecene.

**Type:** air  
**GLP:** Not applicable  
**Year:** Not applicable

#### Results

##### Indirect photolysis

**Sensitiser (type):** OH  
**Rate Constant:** 73.1314 E-12 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 1.755 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>)

**Rate Constant:** 80.7314 E-12 cm<sup>3</sup>/molecule-sec [trans]  
**Degradation % after:** 50% after 1.590 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>) [trans]

**Sensitiser (type):** Ozone  
**Rate Constant:** 13 E-17 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 2.116 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

Rate Constant: 20 E-17 cm<sup>3</sup>/molecule-sec [trans]  
Degradation % after: 50% after 1.375 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

**Reliability:** (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

**Flag:** Critical study for SIDS endpoint

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 26: 2293-99.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### (4) Test Substance

Identity: CAS No. 1120-36-1, 1-Tetradecene

#### Method

Method/  
guideline followed: Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.10 which uses a program described by Meylan, W.M. and Howard, P.H. (1993). Program used the structure for 1-tetradecene.

Type: air  
GLP: Not applicable  
Year: Not applicable

#### Results

##### Indirect photolysis

Sensitiser (type): OH  
Rate Constant: 41.4824 E-12 cm<sup>3</sup>/molecule-sec  
Degradation % after: 50% after 3.094 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>)

Sensitiser (type): Ozone  
Rate Constant: 1.2 E-17 cm<sup>3</sup>/molecule-sec [cis]  
Degradation % after: 50% after 22.90 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

**Reliability:** (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust

summary has a rating of 2 because the data are calculated and not measured.

**Flag:** Critical study for SIDS endpoint

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 26: 2293-99.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(5) **Test Substance**

**Identity:** CAS No.26952-13-6, Tetradecene

**Method**

**Method/  
guideline followed:** Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.10 which uses a program described by Meylan, W.M. and Howard, P.H. (1993). Program used the structure for 2-tetradecene.

**Type:** air  
**GLP:** Not applicable  
**Year:** Not applicable

**Results**

Indirect photolysis

**Sensitiser (type):** OH  
**Rate Constant:** 70.3053 E-12 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 1.826 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>)  
**Rate Constant:** 77.9053 E-12 cm<sup>3</sup>/molecule-sec [trans]  
**Degradation % after:** 50% after 1.648 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>) [trans]

**Sensitiser (type):** Ozone  
**Rate Constant:** 13 E-17 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 2.116 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)  
**Rate Constant:** 20 E-17 cm<sup>3</sup>/molecule-sec [trans]  
**Degradation % after:** 50% after 1.375 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

**Reliability:** (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust

summary has a rating of 2 because the data are calculated and not measured.

**Flag:** Critical study for SIDS endpoint

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 26: 2293-99.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**(6) Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

**Method/  
guideline followed:** Calculated values using AOPWIN version 1.90, a subroutine of the computer program EIPWIN version 3.10 which uses a program described by Meylan, W.M. and Howard, P.H. (1993). Program used the structure for 2-pentadecene.

**Type:** air  
**GLP:** Not applicable  
**Year:** Not applicable

**Results**

**Indirect photolysis**

**Sensitiser (type):** OH  
**Rate Constant:** 71.7184 E-12 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 1.790 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>)  
**Rate Constant:** 79.3184 E-12 cm<sup>3</sup>/molecule-sec [trans]  
**Degradation % after:** 50% after 1.618 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm<sup>3</sup>) [trans]

**Sensitiser (type):** Ozone  
**Rate Constant:** 13 E-17 cm<sup>3</sup>/molecule-sec [cis]  
**Degradation % after:** 50% after 2.116 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)  
**Rate Constant:** 20 E-17 cm<sup>3</sup>/molecule-sec [trans]  
**Degradation % after:** 50% after 1.375 hrs (using avg. ozone conc. of 7 E11 mol/cm<sup>3</sup>)

**Reliability:** (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust

summary has a rating of 2 because the data are calculated and not measured.

**Flag:** Critical study for SIDS endpoint

**References:** Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 26: 2293-99.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## B. Stability in Water

### Test Substance

**Identity:** CAS No. 629-73-2, 1-Hexadecene; CAS No. 26952-14-7, Hexadecene; CAS No. 27251-68-9, Pentadecene; CAS No. 1120-36-1, 1-Tetradecene; or CAS No.26952-13-6, Tetradecene

### Method

**Method/  
guideline followed:** Other – Technical Discussion

**Type (test type):**

**GLP:** Yes [ ] No [ ]

**Year:**

**Test Conditions:** Not applicable

**Results:** Not applicable

**Remarks:** Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H<sub>2</sub>O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (Harris, 1982b) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Higher Olefins Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

The substances in the Higher Olefins Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Higher Olefins Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

**Conclusions:** In the environment, hydrolysis will not contribute to the degradation of C14-C16 alpha or internal olefins.

**Reliability:** Not applicable

**References:** Gould, E.S. (1959) Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982b) "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W. B. (1985) Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

## **C. Stability In Soil**

No data available

### **3.2 Monitoring Data (Environment)**

No data available.

### **3.3 Transport and Distribution**

#### **3.3.1 Transport between environmental compartments**

**A. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Type:** Fugacity models, Mackay Levels I and III

**Remarks:** Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

**Chemical assumptions:**

Molecular weight: 224  
Water solubility: 0.00144 g/m<sup>3</sup>  
Vapor pressure: 0.352 Pa (25°C)  
Log Kow: 8.06  
Melting point: 4.1°C  
Environment name: EQC Standard Environment

Half-life in air = 4.625 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

**Results** Media: Air, soil, water and sediment concentrations were estimated

	<b>Level I</b>	<b>Level III</b>
<b>Air</b>	9.6%	<1%
<b>Water</b>	<1%	7.9%
<b>Soil</b>	88.4%	22.4%
<b>Sediment</b>	2%	69.4%

**Remarks:** Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that 1-hexadecene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Input data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia

Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## B. Test Substance

Identity: CAS No. 26952-14-7, Hexadecene

### Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

#### Chemical assumptions:

Molecular weight: 224  
Water solubility: 0.00144 g/m<sup>3</sup>  
Vapor pressure: 1.18 Pa (25°C)  
Log Kow: 7.98  
Melting point: 0.21°C  
Environment name: EQC Standard Environment

Half-life in air = 1.32 hr, half-life in water = 208 hr, half-life in soil = 208 hr, half-life in sediment = 832 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

**Results** Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
<b>Air</b>	30.6%	<1%
<b>Water</b>	<1%	12.7%
<b>Soil</b>	67.8%	21.0%
<b>Sediment</b>	1.5%	66.1%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that hexadecene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Input data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

### C. Test Substance

**Identity:** CAS No. 27251-68-9, Pentadecene

#### Method

**Type:** Fugacity models, Mackay Levels I and III

**Remarks:** Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

#### Chemical assumptions:

Molecular weight: 210.41  
Water solubility: 0.0045 g/m<sup>3</sup>  
Vapor pressure: 2.61 Pa (25°C)  
Log Kow: 7.49  
Melting point: 11.04°C  
Environment name: EQC Standard Environment

Half-life in air = 1.33 hr, half-life in water = 208 hr, half-life in soil = 208 hr, half-life in sediment = 832 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

#### Results

Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
<b>Air</b>	46.8%	<1%
<b>Water</b>	<1%	12.9%
<b>Soil</b>	52.0%	21.6%
<b>Sediment</b>	1.2%	65.4%

**Remarks:** Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that 1-pentadecene will partition equally to air and soil under equilibrium conditions (Level I model), but primarily to soil and sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Input data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### D. Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

#### Method

**Type:** Fugacity models, Mackay Levels I and III

**Remarks:** Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

#### Chemical assumptions:

Molecular weight: 196.38  
Water solubility: 0.0135 g/m<sup>3</sup>  
Vapor pressure: 1.20 Pa (25°C)  
Log Kow: 7.08  
Melting point: -12°C  
Environment name: EQC Standard Environment

Half-life in air = 4.87 hr, half-life in water = 360 hr, half-life in soil = 360 hr,  
half-life in sediment = 1440 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

**Results** Media: Air, soil, water and sediment concentrations were estimated

	<b>Level I</b>	<b>Level III</b>
<b>Air</b>	24.4%	<1%
<b>Water</b>	<1%	8.52%
<b>Soil</b>	73.9%	24.0%
<b>Sediment</b>	1.64%	67.2%

**Remarks:** Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that 1-tetradecene will partition primarily to soil under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Input data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## E. Test Substance

**Identity:** CAS No.26952-13-6, Tetradecene

### Method

**Type:** Fugacity models, Mackay Levels I and III

**Remarks:** Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000)

#### Chemical assumptions:

Molecular weight: 196.38  
 Water solubility: 0.0139 g/m<sup>3</sup>  
 Vapor pressure: 6.31 Pa (25°C)  
 Log Kow: 7.00  
 Melting point: 0.41°C  
 Environment name: EQC Standard Environment

Half-life in air = 1.34 hr, half-life in water = 208 hr, half-life in soil = 208 hr, half-life in sediment = 832 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

**Results** Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
<b>Air</b>	66.5%	<1%
<b>Water</b>	<1%	13.7%
<b>Soil</b>	32.7%	23.1%
<b>Sediment</b>	<1%	63%

**Remarks:** Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

**Conclusions:** These results indicated that tetradecene will partition primarily to air under equilibrium conditions (Level I model), but primarily to sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

**Reliability:** (2) Valid with restrictions: Input data are calculated.

**Flag:** Critical study for SIDS endpoint

**References:** Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)

EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## F. Test Substance

**Identity:** CAS No. 629-73-2, 1-Hexadecene

### Method

**Type:** Volatilization from water

**Remarks:** Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 6.1 atm-m<sup>3</sup>/mole (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values

**Results:** Half-life from a model river: 1.529 hrs  
Half-life from a model lake: 5.9 days

**Reliability:** (2) Valid with restrictions. Input data were calculated.

**References:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**G. Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

**Method**

**Type:** Volatilization from water

**Remarks:** Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of  $7.2 \text{ atm}\cdot\text{m}^3/\text{mole}$  (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values

**Results:** Half-life from a model river: 1.529 hrs  
Half-life from a model lake: 5.9 days

**Reliability:** (2) Valid with restrictions. Input data were calculated.

**References:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**H. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

**Type:** Volatilization from water

**Remarks:** Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of  $5.42 \text{ atm}\cdot\text{m}^3/\text{mole}$  (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values

**Results:** Half-life from a model river: 1.48 hrs  
Half-life from a model lake: 5.741 days

**Reliability:** (2) Valid with restrictions. Input data were calculated.

**References:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**I. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Type:** Volatilization from water

**Remarks:** Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 9.69 atm-m<sup>3</sup>/mole (calculated by EPIWIN from vapor pressure [0.015 mm Hg] and water solubility [0.0004 ppm]) and EPIWIN default values

**Results:** Half-life from a model river: 1.43 hrs  
Half-life from a model lake: 5.546days

**Reliability:** (2) Valid with restrictions. Input data were calculated.

**References:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**J. Test Substance**

**Identity:** CAS No.26952-13-6, Tetradecene

**Method**

**Type:** Volatilization from water

**Remarks:** Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 4.08 atm-m<sup>3</sup>/mole (estimated by Bond SAR method using HENRYWIN program) and EPIWIN default values

**Results:** Half-life from a model river: 1.43 hrs  
Half-life from a model lake: 5.546 days

**Reliability:** (2) Valid with restrictions. Input data were calculated.

**References:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**3.3.2 Distribution**

**A. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene or CAS No. 26952-14-7, Hexadecene

**Method**

**Method:** Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, based on the method of Meylan et al., 1992.

**Test Conditions:** Based on chemical structure

**Results**

**Value:** Estimated Koc = 6.79e+004

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

**Method:** Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, based on the method of Meylan et al., 1992.

**Test Conditions:** Based on chemical structure

**Results**

**Value:** Estimated Koc = 36790

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene; or CAS No.26952-13-6, Tetradecene

**Method**

**Method:** Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, based on the method of Meylan et al., 1992.

**Test Conditions:** Based on chemical structure

**Results**

**Value:** Estimated Koc = 19950

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

**Method**

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 0.00264 mm Hg and WS = 0.00144 mg/L.

**Results**

**Value:** Bond estimate = 6.10 atm-m<sup>3</sup>/mole  
Group estimate = 16.9 atm-m<sup>3</sup>/mole  
VP/Wsol estimate = 0.541 atm-m<sup>3</sup>/mole

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

**Method**

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 0.00887 mm Hg and WS = 0.00144 mg/L.

**Results**

**Value:** Bond estimate = 7.20 atm-m<sup>3</sup>/mole  
Group estimate = 11.7 atm-m<sup>3</sup>/mole  
VP/Wsol estimate = 1.82 atm-m<sup>3</sup>/mole

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**F. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Method**

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 0.0196 mm Hg and WS = 0.00448 mg/L.

**Results**

**Value:** Bond estimate = 5.42 atm-m<sup>3</sup>/mole  
Group estimate = 8.29 atm-m<sup>3</sup>/mole  
VP/Wsol estimate = 1.21 atm-m<sup>3</sup>/mole

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**G. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 0.015 mm Hg and WS = 0.0004 mg/L.

## Results

**Value:** Bond estimate = 3.46 atm-m<sup>3</sup>/mole  
Group estimate = 8.48 atm-m<sup>3</sup>/mole  
VP/Wsol estimate = 9.69 atm-m<sup>3</sup>/mole

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## H. Test Substance

**Identity:** CAS No.26952-13-6, Tetradecene

### Method

**Method:** Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

**Test Conditions:** Bond and Group estimates based on chemical structure, at 25°C;  
VP/water solubility estimates based on EPIWIN values of VP = 0.0473 mm Hg and WS = 0.0139 mg/L.

## Results

**Value:** Bond estimate = 4.08 atm-m<sup>3</sup>/mole  
Group estimate = 5.87 atm-m<sup>3</sup>/mole  
VP/Wsol estimate = 0.88 atm-m<sup>3</sup>/mole

**Reliability:** (2) Reliable with restrictions. Value is calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## 3.4 Aerobic Biodegradation

### A. Test Substance

**Identity:** CAS No. 629-73-2, 1-Hexadecene

### Method

**Method/guideline:** OECD 301C, Ready Biodegradability, Modified MITI Test (I)  
**Type:** Aerobic [X] Anaerobic [ ]  
**GLP:** no data  
**Year:** no data

**Contact time:** 28 days  
**Inoculum:** Mixture from several sources in Japan that included 4 sewage plants, 3 rivers, 2 bays, and 1 lake.

**Test Conditions:** A mixed inoculum was developed and maintained that used ten sources and included: return sludge from 1 industrial and 3 city sewage plants; and water from 3 rivers, 2 bays, and 1 lake, with soil from land adjacent to these bodies of water. A filtrate from the combination of these samples was prepared and added to an existing culture that had been developed from the same sources as above and maintained under aeration and with a synthetic feed composed of glucose, peptone, and monopotassium phosphate. The inoculum used for this biodegradation test was removed from the mixed culture and added to the test systems at a concentration of 30 mg of inoculum per liter of test medium. Blank and positive controls were used per guideline. The positive control, aniline, was added to the control vessel at a loading rate of 100 mg/L. Test systems contained 100 mg test substance per liter of medium (3 replicates). The volume of test solution was 300 ml. Temperature of incubation: 24 - 26°C. Oxygen consumption was monitored using a closed system oxygen consumption measuring apparatus from Ohkura Electric Co., Ltd. Percent biodegradation was calculated as a percent ratio of the biological oxygen demand (BOD) in the test system less the BOD of the blank control, to the calculated theoretical oxygen demand of the added test material. When percentage biodegradations of aniline calculated by BOD value were beyond 40% and 60% at the 7th and 14th day, respectively, it was concluded that the test condition was valid.

**Results:** Readily biodegradable: The degree of biodegradation of the test material was 55 – 77% after 28 days.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	55, 77, 73	68

\* replicate data

By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted.

**Reliability:** (2) Reliable with restrictions: Reference compound data are not presented and the range in biodegradation values is not less than 20% as required in OECD guideline 301C.

**Flag:** Key study for SIDS endpoint

**Reference:** Chemicals Inspection and Testing Institute, Japan (1992) Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology and Information Center.

## B. Test Substance

**Identity:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

### Method

**Method/guideline:** ISO "Marine BODIS" ISO/TC 147/SC 5/WG 4N 1415  
**Type:** Aerobic [X ] Anaerobic [ ]  
**GLP:** No  
**Year:** 1995  
**Contact time:** 28 days  
**Inoculum:** None

**Test Conditions:** This method used natural seawater fortified with mineral nutrients and no inoculum was added in addition to the microorganisms already present in the seawater.

The test vessels were closed glass bottles with a known volume of aqueous test mixture (66.6%) and air (33.3%). They were shaken continuously to assure steady state oxygen partitioning between the aqueous and gaseous phase. The degradation was followed by weekly measurements of the BOD in the aqueous phase for a 28-day period. The test vessels were re-aerated and resealed after measurement. The total oxygen uptake in the test flasks was calculated from the measured oxygen concentration divided by the saturation value at normal conditions and multiplied with the total oxygen content originally present in the aqueous and gaseous phases.

Three replicates were used for each test condition: test substance, controls, and insoluble reference substance. The total oxygen capacity of each test vessel was 26.64 mg oxygen. Sodium benzoate was used as the soluble reference substance at a concentration of 20 mg of theoretical oxygen demand (ThOD) per test vessel.

An inert support medium, chromatography silica powder, was used to provide a large and controlled surface area for the poorly-soluble test substance and reference substance (an olefin oil) The silica powder) and test material were made into a homogenate and added to the test vessel before addition of the test medium. One gram of support medium containing 20 mg of ThOD of test substance or insoluble reference substance was used for each test vessel. The ThOD for the test substance was 0.34 mg oxygen/mg and the addition rate was 4 mg/test vessel.

The following controls were included: Background oxygen consumption in test medium, background oxygen consumption in test medium with clean silica powder.

Validity criteria stated: Temperature = 19-21°C, Soluble reference is >60% in 14 days, and Cumulative blank oxygen consumption is <30% of

oxygen initially available. The Reference insoluble material is expected to achieve 25-45% in 28 days.

**Results:** The test material achieved 48% biodegradation in 28 days.

**Kinetic of  
Test substance:**  
7 day = 19 %  
14 day = 31 %  
21 day = 44 %  
28 day = 48 %

**Kinetic of control  
Substance  
(Sodium benzoate):**  
14 day = 58 %  
28 day = 85 %

**Reliability:** (2) Reliable with restrictions: This study does not meet the validity criteria stated in the report. The Soluble reference, sodium benzoate only achieved 58% degradation by Day 14, instead of 60%.

**Reference:** Environment & Resource Technology Ltd. (1999) Assessment of ready aerobic degradability of C16/C18 isomerized olefin base fluid in seawater. Study No. 074-9. Conducted for Chevron Chemical Company (unpublished report).

### C. Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene; CAS No.26952-13-6, Tetradecene ; CAS No. 27251-68-9, Pentadecene; CAS No. 629-73-2, 1-Hexadecene; or CAS No. 26952-14-7, Hexadecene

#### Method

**Method/guideline:  
Type:** Estimated using the computer program EPIWIN v 3.11, BIOWIN v 4.01  
Aerobic

**Test Conditions:** Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

**Results:** Linear model prediction: Biodegrades fast  
Non-linear model prediction: Biodegrades fast  
Ultimate biodegradation timeframe: Weeks (for C14 and C16 alpha olefins) or days-weeks for the other olefins

Primary biodegradation timeframe: Days  
MITI linear model prediction: Biodegrades fast  
MITI non-linear model prediction: Biodegrades fast

**Reliability:** (2) Reliable with restriction: Results are estimated

**Flag:** Key study for SIDS endpoint

**Reference:** Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

**Identity:** CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

**Method**

**Method/guideline:** Estimated using the computer program EPIWIN v 3.11, BIOWIN v 4.01  
**Type:** Aerobic

**Test Conditions:** Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

**Results:** Linear model prediction: Biodegrades fast  
Non-linear model prediction: Biodegrades fast  
Ultimate biodegradation timeframe: Days-Weeks  
Primary biodegradation timeframe: Days-weeks  
MITI linear model prediction: Does not biodegrade fast  
MITI non-linear model prediction: Does not biodegrade fast

**Reliability:** (2) Reliable with restriction: Results are estimated

**Flag:** Key study for SIDS endpoint

**Reference:** Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### **E. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene – 98%

#### **Method**

**Method/guideline:** OECD 301D  
**Type:** Aerobic [X ] Anaerobic [ ]  
**GLP:** Yes  
**Year:** 1985  
**Contact time:** 28 days  
**Inoculum:** Prepared according to guideline

**Test Conditions:** Test substance was emulsified with Dobane PT sulphonate. The test concentration was 2 mg 1-tetradecene/L.

**Results:** 1-Tetradecene was degraded with 62-65% of the theoretical 28-day oxygen demand.

**Kinetic:**  
5 day = 47-51%  
15 day = 80-87%  
28 day = 62-65%

**Remarks:** The apparent discrepancy between 15-day and 28-day values was explained by increased oxygen uptake in the blanks only.

**Reliability:** (2) Reliable with restrictions: It is not known whether the results met the 10 day window requirement of the testing guideline. Only limited information was available.

**Reference:** Turner, S.J. and Watkinson, R.J. (1985) 1-Tetradecene: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

## F. Test Substance

Identity: CAS No. 1120-36-1, 1-Tetradecene – 98%

### Method

Method/guideline: OECD 301B Modified Sturm

Type: Aerobic [X] Anaerobic [ ]

GLP: Yes

Year: 1985

Contact time: 28 days

Inoculum: Prepared according to guideline

**Test Conditions:** Test substance was emulsified with Dobane PT sulphonate. The test concentration was 20 mg 1-tetradecene/L.

**Results:** 1-Tetradecene was degraded with 48-56% after 28 days

**Reliability:** (2) Reliable with restrictions: Only limited information was available.

**Reference:** Turner, S.J. and Watkinson, R.J. (1985) 1-Tetradecene: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

## 3.5 BOD5, COD or ratio BOD5/COD

No data available

## 3.6 Bioaccumulation

### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene

### Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and Log Kow (estimated as 8.06 by EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = -1.37 \log \text{Kow} + 14.4 + \text{correction}$  (alkyl chains [8+ -CH<sub>2</sub>- groups] with a value of -1.5).

### Results

**Value:** Estimated Log BCF = 1.854 (BCF = 71.49)

**Reliability:** (2) Reliable with restrictions. Value was calculated.

**Reference:** Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## **B. Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

### **Method**

**Method:** BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and Log Kow (estimated as 7.98 by EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = -1.37 \log \text{Kow} + 14.4 + \text{correction}$  (alkyl chains [8+ -CH<sub>2</sub>- groups] with a value of -1.5).

### **Results**

**Value:** Estimated Log BCF = 1.962 (BCF = 91.61)

**Reliability:** (2) Reliable with restrictions. Value was calculated.

**Reference:** Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

## **C. Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

### **Method**

**Method:** BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and Log Kow (estimated as 7.49 by EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = -1.37 \log \text{Kow} + 14.4 + \text{correction}$  (alkyl chains [8+ -CH<sub>2</sub>- groups] with a value of -1.5).

**Results**

**Value:** Estimated Log BCF = 2.635 (BCF = 431.2)

**Reliability:** (2) Reliable with restrictions. Value was calculated.

**Reference:** Meylan, WM, Howard, PH, Boethling, RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method:** BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and Log Kow (estimated as 7.08 by EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = -1.37 \log \text{Kow} + 14.4 + \text{correction}$  (alkyl chains [8+ -CH<sub>2</sub>- groups] with a value of -1.5).

**Results**

**Value:** Estimated Log BCF = 3.200 (BCF = 1584)

**Reliability:** (2) Reliable with restrictions. Value was calculated.

**Reference:** Meylan, WM, Howard, PH, Boethling, RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Test Substance**

**Identity:** CAS No.26952-13-6, Tetradecene

**Method**

**Method:** BCF calculated value using the computer program EPIWIN, BCF v 2.15

**Test Conditions:** Based on chemical structure and Log Kow (estimated as 7.00 by EPIWIN) using methods described by Meylan et al., 1999. Formula used to make BCF estimate:  $\text{Log BCF} = -1.37 \log \text{Kow} + 14.4 + \text{correction}$  (alkyl chains [8+ -CH<sub>2</sub>- groups] with a value of -1.5).

**Results**

**Value:** Estimated Log BCF = 3.308 (BCF = 2030)

**Reliability:** (2) Reliable with restrictions. Value was calculated.

**Reference:** Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672.

EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**3.7 Additional Information**

**A. Sewage Treatment**

**Test Substance**

**Identity:** CAS No: 629-73-2, 1-Hexadecene

**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 224.43; VP = 0.00264 mmHg; Henry's LC = 6.1 atm-m<sup>3</sup>/mol; air-water partition coefficient = 249.472; Log Kow = 8.06; biomass to water partition coefficient = 2.29631E+007; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 96.99 % removed from wastewater treatment

**Reliability:** (2) Reliable with restrictions: Value was calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**B. Sewage Treatment**

**Test Substance**

**Identity:** CAS No. 26952-14-7, Hexadecene

**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 224.43; Henry's LC = 7.2 atm·m<sup>3</sup>/mol; air-water partition coefficient = 294.459; Log Kow = 7.98; biomass to water partition coefficient = 1.90999E+007; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 97.51 % removed from wastewater treatment

**Reliability:** (2) Reliable with restrictions: Value was calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**C. Sewage Treatment**

**Test Substance**

**Identity:** CAS No. 27251-68-9, Pentadecene

**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 210.41; Henry's LC = 5.42 atm·m<sup>3</sup>/mol; air-water partition coefficient = 221.662; Log Kow = 7.49; biomass to water partition coefficient = 6.18059 E+006; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 99.58 % removed from wastewater treatment

**Reliability:** (2) Reliable with restrictions: Value was calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**D. Sewage Treatment**

**Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 196.38; VP = 0.015 mmHg; Henry's LC = 9.68977 atm-m<sup>3</sup>/mol; air-water partition coefficient = 396.283; Log Kow = 7.08; biomass to water partition coefficient = 2.40453E+006; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 99.61 % removed from wastewater treatment

**Reliability:** (2) Reliable with restrictions: Value was calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

**E. Sewage Treatment**

**Test Substance**

**Identity:** CAS No.26952-13-6, Tetradecene

**Test Method:** Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

**Input values:** MW = 196.38; Henry's LC = 4.08 atm-m<sup>3</sup>/mol; air-water partition coefficient = 166.86; Log Kow = 7.00; biomass to water partition coefficient = 2E+006; temperature = 25°C

**GLP:** No

**Test Medium:** Secondary waste water treatment (water)

**Test Type:** Aerobic

**Test Results:** 99.28 % removed from wastewater treatment

**Reliability:** (2) Reliable with restrictions: Value was calculated.

**Reference:** EPIWIN (2000) Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

#### 4. ENVIRONMENTAL TOXICITY

##### 4.1 Acute Toxicity to Fish

###### A. Test Substance

**Identity:** CAS No. 629-73-2, 1-Hexadecene (~93%, GULFTENE 16)

###### Method

**Method/guideline:** OECD 203

**Test type:** Semi-static Fish Acute Toxicity Test

**GLP:** Yes [X] No [ ]

**Year:** 1993

**Species/Strain:** *Oncorhynchus mykiss* (Rainbow trout)

**Analytical Monitoring:** Water samples were taken from the control and each exposure level at 0 hours for test concentration verification. The concentrations were analyzed using an Ionics TC/TOC Analyser Model 555. The analytical detection limit was not reported. Since the values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than the control level, analysis was not carried out at other time points.

**Exposure period:** 96 hours

**Statistical methods:** Not specified

**Test Conditions:** A study was performed to assess the acute toxicity of GULFTENE 16 to rainbow trout (*Oncorhynchus mykiss*) under semistatic conditions (daily renewal).

The water accommodated fraction (WAF) was prepared by mixing 1000 mg/l GULFTENE 16 with water. The mixture was stirred on magnetic stirrers for 24 hours at 14°C and then allowed to settle for approximately 1 hour. The WAF was then withdrawn via a siphon prior to dilution to the required exposure levels and testing.

The test water was laboratory tap water (filtered, dechlorinated and softened; hardness =  $164 \pm 9$  mg CaCO<sub>3</sub>/L; alkalinity = 210). Test temperature was 13-14°C. Photoperiod was 16 h light and 8 h dark. pH ranged from 7.7 to 8.1. Dissolved oxygen ranged from 9.9 to 10 mg O<sub>2</sub>/L.

Groups of ten juvenile fish (5 test concentrations plus one control) were exposed for 96 hours to a dilution series of a single WAF of GULFTENE 16 (100 % WAF equivalent to 1000 mg/L). The size of the control fish at the end of the exposure period was  $5.1 \pm 0.5$  cm and the weight was  $1.73 \pm$

0.51 g. Supplementary aeration was provided. The test concentrations were 10, 18, 32, 56, and 100% WAF. Observations were made on the numbers of dead fish and the incidence of sub-lethal effects after 3, 6, 24, 72 and 96 hours exposure.

**Results:** The 96-hour LC50 was > solubility; LL0 = 1000 mg/L loading rate WAF.

The NOEC was 1000 mg/L loading rate WAF.

**Remarks:** There were no mortalities or sub-lethal effects. Values obtained at 0 hours demonstrated that Total Carbon (dissolved) values (TOC) for the exposure media were no higher than that of the control level. TOC values for the experimental medium were 21.0-22.5 mg/L vs 23.0 mg/L for the control. The actual concentration was negligible.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Huntingdon Research Centre (1993) GULFTENE 16 (water accommodated fraction) acute toxicity to rainbow trout, Study No. CHR 47(a)/930363. Conducted for Chevron Research and Technology Company (unpublished report).

## B. Test Substance

**Identity:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

### Method

**Method/guideline:** OECD 203  
**Test type:** Semistatic Fish Acute Toxicity Test  
**GLP:** Yes [X] No [ ]  
**Year:** 1995  
**Species/Strain:** *Scophthalmus maximus*  
**Analytical Monitoring:** no  
**Exposure period:** 96 hours  
**Statistical methods:** Not specified

**Test Conditions:** Based on range-finding data, the definitive test (semi-static) was conducted on 5 dose levels (loading levels of 1000, 1800, 3200, 5600, and 10000) and a control. Actual concentrations in test media were not measured. Juvenile turbot of approximately 3cm in length were used in all tests. Fish supplied by Mannin Seafarms Ltd. (Scotland) were maintained in controlled conditions of approximately 18 °C with constant illumination. The pH ranged from 7.8 to 8.3. The dissolved

oxygen ranged from 85% to 98%. The tests were conducted in 14L capacity moulded soda-lime glass tanks containing 10 liters of test media (1 µm filtered UV treated seawater) . The test material was added directly to the appropriate tank and the test media was replaced at 48 hours. A single vessel was used per test concentration and gentle aeration was supplied. Ten animals were exposed per test concentration for 96 hours with observations being conducted at 24 hour intervals.

**Results:** After 96 hours, no mortality was observed at the maximum dose level of 10,000 mg/L (loading levels), therefore, the LC50 was greater than solubility and the LL0 was 10,000 mg/L. The actual concentration was negligible.

**Reliability:** (2) Reliable with restrictions. The study was conducted under GLPs and can be considered a guideline study. However, The substance was tested at concentrations above the water solubility limit and concentrations were not verified by analysis. Toxicity endpoint was expressed as the initial nominal concentration. Also, constant illumination was used during the study instead of the recommended 12-16 hour photoperiod.

**References:** Environment & Resource Technology Ltd. (1997) Assessment of the aquatic-phase toxicity of C16-C18 Alpha Olefin to the marine fish, *Scophthalmus maximus*, Study No. 074-5-1. Conducted for Chevron Chemical Company (unpublished report).

### C. Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Remarks:** Test articles from three suppliers were blended to produce the final test article consisting of 99% 1-tetradecene.

### Method

**Method/guideline:** OECD 203

**Test type:** 96 hour semistatic toxicity test

**GLP:** Yes

**Year:** 1995

**Species/Strain:** Rainbow trout (*Oncorhynchus mykiss*)

**Analytical Monitoring:** Total organic carbon (TOC) concentration was measured in a sample taken from each treatment and control solution, prior to addition of the fish. The TOC concentrations were measured with a Shimadzu Model TOC-5000 analyzer.

**Exposure period:** 96 hr

**Statistical methods:** The 96 hr LC50 value was estimated by visual inspection of the mortality data.

**Test Conditions:** Water-accommodated fractions (WAFs) were prepared by adding the appropriate amount of 1-tetradecene to dilution water on a weight-volume basis. The WAFs were mixed for 24 hours inside a covered

glass vessel using a magnetic stirrer at a speed that produced a vortex extending 30-50% from the surface to the bottom of the vessel. After the mixing period, the mixture was allowed to settle for one hour before the water phase containing the WAF was siphoned off and used as the test solution. Test solutions were renewed daily using freshly prepared WAFs.

Fish eggs were supplied by Mt. Lassen Trout Farm, Red Bluff, CA; hatched at Wildlife International; and held for approximately 41 days prior to the definitive test. The average length of 7 negative control fish measured at the end of the definitive test was 31 mm with a range of 29-32 mm. The average wet weight of 7 negative control fish at the end of the test was 0.38 g with a range of 0.33 – 0.45 g. Loading = 0.90 g/L.

The water used for culturing and testing was freshwater from a well on the laboratory site. Zero-hour dilution water measurements: conductivity = 305-310  $\mu$  S/cm; hardness = 128 mg/L as CaCO<sub>3</sub>; alkalinity = 176-178 mg/L as CaCO<sub>3</sub>. The temperature measured continuously during the test ranged from 14.0 – 16.5 °C. Light intensity at test initiation was approximately 911 lux at the surface of the water (photoperiod: 16 hrs light and 8 hrs darkness). On Day 1, dissolved oxygen concentrations dropped as low as 5.2 mg/L (52% of saturation). All other dissolved oxygen concentrations measured were above 60% of saturation. pH = 7.6-8.4.

The range finding test used test concentrations of WAFs from 10, 100, and 1000 mg test article per liter, and five fish per chamber. No deaths were seen during the range finding test.

A definitive limit test was then conducted using 7 fish per chamber and two replicates each in the control and treatment (WAF from 1000 mg/L) groups.

**Results:**

LC<sub>50</sub> (96 hr) > solubility

LL0 = 1000 mg/L (EPA reviewed for SIAM 11)

**Remarks:**

No deaths or abnormal signs were noted at any time point in the control or treated groups. Test organisms appeared normal and healthy throughout the test. The 96-hour LC50 was thus greater than WAF from 1000 mg test article/liter.

LL0 = lethal loading based on the WAF testing procedure, no mortality observed at the highest loading indicated.

Measurement of TOC ranged from less than the limit of detection (0.5 mg/L) to 1.4 mg/L. Based on the acceptable precision of TOC measurements at Wildlife International ( $\pm$ 15%), WAFs of 1-tetradecene were indistinguishable from untreated control water.

**Reliability:**

(1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint

**References:** Drottar, L.R., and Swigert, J.P. (1995) 1-Tetradecene: A Water-Accommodated Fraction 96-hour Semistatic Acute Toxicity Test with the Rainbow Trout (*Oncorhynchus mykiss*). Conducted by Wildlife International Ltd., Easton, Maryland, Report No. 398A-102A. for the Chemical Manufacturers Association, Alpha Olefins Panel, Sponsor (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

## 4.2 Acute Toxicity to Aquatic Invertebrates (e.g. *Daphnia*)

### Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Remarks:** Blend of three suppliers' 1-tetradecene, 99% purity

### Method

**Method/guideline:** OECD 202, Part 1

**Test type:** Semi-static

**GLP:** Yes

**Year:** 1995

**Analytical Monitoring:** Total organic carbon (TOC) concentration was measured in a sample taken from each treatment and control solution, prior to addition of the daphnids. The TOC concentrations were measured with a Shimadzu Model TOC-5000 analyzer. The limit of detection was 0.5 mg/L.

**Species/Strain:** *Daphnia magna*

**Exposure period:** 48 hrs

**Statistical methods:** The 48 hr EC50 value was estimated by visual inspection of the mortality/immobility data.

**Test Conditions:** This study was a semi-static study using a water-accommodating fraction (WAF) of test article. Water-accommodated fractions (WAFs) were prepared by adding the appropriate amount of 1-tetradecene to dilution water on a weight-volume basis. The WAFs were mixed for 24 hours inside a covered glass vessel using a magnetic stirrer at a speed that produced a vortex extending 30-50% from the surface to the bottom of the vessel. After the mixing period, the mixture was allowed to settle for one hour before the water phase containing the WAF was siphoned off and used as the test solution. Test solutions were renewed on Day-1 of the test using freshly prepared WAFs.

Neonate daphnids used for tests, less than 24 hours old, were obtained from cultures maintained by Wildlife International. The test chambers were 250-ml glass beakers containing approximately 200 ml of test solution. The chambers were covered with plastic wrap.

The water used for culturing and testing was freshwater from a well on the laboratory site. Zero-hour dilution water measurements: conductivity = 340  $\mu\text{mhos/cm}$ ; hardness = 132 mg/L as  $\text{CaCO}_3$ ; alkalinity = 184 mg/L as  $\text{CaCO}_3$ . The temperature measured continuously during the test ranged from 19.5 – 20.5 °C. Light intensity at test initiation was approximately 725 lux at the surface of the water (photoperiod: 16 hrs light and 8 hrs darkness). Dissolved oxygen concentrations were above 60% of saturation. pH = 8.3-8.5.

In the range-finding test, daphnia were exposed to the WAFs prepared from 10, 100, or 1000 mg/L test article in water. No deaths occurred during the range-finding test. The definitive limit test used a single WAF prepared from test article at 1000 mg/L and a negative control (well water). Four replicate test chambers were maintained in the treatment and control groups, with 5 daphnids in each chamber.

**Results:** The 48-hour EC50 for *Daphnia magna* under the conditions of this test was greater than solubility. The ELO was 1000 mg/liter (WAF).

ELO = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated.

**Remarks:** Test organisms in the control group appeared normal and healthy throughout the test. Some organisms in the treatment group appeared to be “floating” but appeared normal when re-submerged with a drop of water. All other organisms appeared normal. Measurement of TOC ranged from 0.6 to 0.7 mg/L. Based on the acceptable precision of TOC measurements at Wildlife International ( $\pm 15\%$ ), WAFs of 1-tetradecene were indistinguishable from untreated control water.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint

**References:** Drottar, L.R., and Swigert, J.P. (1995) 1-Tetradecene: A Water-Accommodated Fraction 48-hour Semistatic Acute Mobilization Test With the Cladoceran (*Daphnia magna*). Conducted by Wildlife International LTD., Easton, Maryland, Report No. 398A-103, for the Alpha Olefins Panel, Chemical Manufacturers Association (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

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

##### A. Test Substance

Identity: CAS No. 629-73-2, 1-Hexadecene (~93%, GULFTENE 16)

##### Method

**Method/guideline:** OECD 201  
**Test type:** static  
**GLP:** Yes [X] No [ ]  
**Year:** 1993  
**Analytical Monitoring:** Water samples were taken from the control and each exposure level at 0 hours for test concentration verification. The concentrations were analyzed using an Ionics TC/TOC Analyser Model 555. Since the values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than the control level, analysis was not carried out at other time points. The limit of detection was not reported.

**Species/Strain:** *Selenastrum capricornutum*  
**Element basis:** Growth rate  
**Exposure period:** 72 hrs  
**Statistical methods:** Not specified

**Test Conditions:** The water accommodated fraction (WAF) was prepared by mixing 1000 mg/L GULFTENE 16 with water. The mixture was stirred on a magnetic stirrer for 24 hours at 24°C and then allowed to settle for approximately 1 hour. The WAF was then withdrawn via a siphon and 100 ml was measured into 250 ml conical flasks. Flasks were prepared and 2 ml of a concentrated algal suspension of *Selenastrum capricornutum* (0.870 absorbance @ 665 nm) were added to each flask in order to produce the correct starting cell density. The flasks were loosely stoppered. Algal cultures were exposed to 6 replicates of a single WAF of GULFTENE 16 (100% WAF equivalent to 1000 mg/L). The exposed cultures plus one control (6 replicates) were incubated without media renewal on an orbital shaker under continuous illumination (~7000 lux) at 24°C for 72 hours. Growth was monitored daily by measuring the absorbance of each culture. The cell densities at initiation and termination for the control were determined by direct counting with a haemocytometer.

**Results:** The 72-hour EbC50 was > solubility; the EbL0 was 1000 mg/L loading rate WAF.  
 The 24-48-hour ErC50 was > solubility; the ErL0 was 1000 mg/L loading rate WAF.  
 The NOEC was 1000 mg/L loading rate WAF.

ELO = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated.

**Remarks:** The mean cell density of the control at 0 hours was  $8.25 \times 10^4$  cells/ml and at 72 hours was  $2.78 \times 10^6$  cells/ml. All test and control cultures were inspected microscopically at 72 hours. There were no abnormalities detected. The values obtained at 0 hours demonstrated that Total Carbon (dissolved) values for the exposure media were no higher than that of the control level. The TOC value for experimental media was 8.05 mg/L vs 8.70 mg/L for the control. The actual concentration was negligible.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint

**References:** Huntingdon Research Centre (1993) GULFTENE 16 (water accommodated fraction) Algal Growth Inhibition, Project No. CHR 47(a)/930363. Conducted for Chevron Research and Technology Company (unpublished report).

**B. Test Substance**

**Identity:** CAS No. 1120-36-1, 1-Tetradecene

**Remarks:** Blend of three supplier's 1-tetradecene, 99% purity

**Method**

**Method/guideline:** OECD 201

**Test type:** static

**GLP:** Yes [X] No [ ]

**Year:** 1995

**Analytical Monitoring:** Total organic carbon (TOC) concentration was measured in a sample taken from each treatment and control solution, prior to addition of the fish. The TOC concentrations were measured with a Shimadzu Model TOC-5000 analyzer. Because TOC could not provide an accurate measurement of the loading of 1-tetradecene in the test water, this analysis was not performed for the definitive test.

**Species/Strain:** *Selenastrum capricornutum*

**Element basis:** Growth rate

**Exposure period:** 96 hrs

**Statistical methods:**

**Test Conditions:** This study was a static study using a water-accommodating fraction (WAF) of test article. Water-accommodated fractions (WAFs) were prepared by adding the appropriate amount of 1-tetradecene to dilution water on a weight-volume basis. The WAFs were mixed for 24 hours inside a covered glass vessel using a magnetic stirrer at a speed that produced a vortex extending 30-50% from the surface to the bottom of the vessel. After the mixing period, the mixture was allowed to settle for one hour before the water phase containing the WAF was siphoned off and used as the test solution.

Algal cells used for tests were obtained from cultures maintained by Wildlife International. Cells less than 24 hours old were obtained from cultures that had been actively growing in culture medium for at least 2 wks prior to test initiation. The test chambers were 250-ml Erlenmeyer flasks containing approximately 100 ml of test solution or control medium. The test flasks were plugged with gauze-wrapped cotton stoppers and shaken continuously at approx. 100 rpm.

Algal cells were cultured and tested in freshwater algal medium [ASTM Standard Guide 1218-90E. Standard Guide for Conducting Static 96-hr Toxicity Tests with microalgae. August 1990]. The water used for culturing and testing was freshwater from a well on the laboratory site. The pH of the medium was adjusted to  $7.5 \pm 0.1$ . The temperatures ranged from 23.5 – 24.5 °C. Light intensity (continuous cool-white fluorescent) ranged from 6400 – 8270 lux. pH was 7.4 at 0 hrs and 8.7 and 8.3 for the treatment and control group, respectively, at 96 hrs.

At test initiation, an inoculum of the algal cells was prepared at a concentration of approx.  $1.0 \times 10^6$  cells/ml. The concentration was verified and 1.0 ml was added to each test chamber to achieve a nominal concentration of approx. 10,000 cells/ml.

Two range-finding tests were conducted. The first used WAFs from 10, 100 and 1000 mg/L, and the second used WAFs from 1.0, 5.0, 10, 100, and 1000 mg/L. The second test showed less than 50% inhibition of algal biomass at each treatment level.

A definitive limit test was conducted with a single WAF (from 1000 mg/L) and a culture medium negative control. Cell densities were used to calculate area under the growth curve values, which were subsequently used to calculate percent inhibition values relative to the control over the 96-hour exposure period. Cell counts were conducted using a hemacytometer and microscope. EBC 50 values (the theoretical toxicant concentrations that would produce a 50% reduction in algal biomass) were determined for 72 and 96 hours of exposure.

Experimental design (definitive test): a single WAF of 1000 mg/L, and a negative (culture medium) control; 6 replicate test chambers for the negative control and 3 replicate test chambers for the treatment group.

Cell densities, area under the growth curve values and percent inhibition values were calculated using "Lotus 1-2-3, Release 3.1" [Lotus Development Corp., copyright 1990]

**Results:** 72 and 96-hr  $E_bC_{50}$  > solubility;  $EL_0$  = 1000 mg/L (nominal)

**Remarks:**  $E_bC_{50}$  values determined for 72 and 96 hours of exposure were determined to be greater than the water accommodating fraction from 1000 mg/L.

$EL_0$  = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated.

Measurement of TOC ranged from less than the limit of detection (LOD) of 0.5 mg/L to 10.4 mg/L in the initial rangefinding test, and from <LOD of 1.0 mg/L to 1.2 mg/L in the second rangefinding test. Actual concentration was negligible.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint

**References:** Thompson, S.G., and Swigert, J.P. (1995) 1-Tetradecene: A Water-Accommodating Fraction 96-hour Toxicity Test with the Freshwater Alga (*Selenastrum capricornutum*). Conducted by Wildlife International, Ltd., Easton, Maryland, Report No. 398A-101, for Chemical Manufacturers Association, Alpha Olefins Panel (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

#### 4.4 Toxicity to Micro-organisms, e.g. Bacteria

##### A. Test Substance

**Identity:** CAS No. 1120-36-1, 1-Tetradecene (98%)

##### Method

**Method:** FMB SOP 021  
**GLP:** No  
**Species:** *Pseudomonas fluorescens*  
**Exposure Period:** 6 hours  
**Analytical Monitoring:** No data

**Results:** EC50 >1000 mg/L

**Reliability:** (2) Reliable with restrictions: comparable to guideline study with acceptable restrictions

**Reference:** Turner, S.J. and Watkinson, R.J. (1985) 1-Tetradecene: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne, UK (unpublished report)

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

##### B. Test Substance

**Identity:** CAS No. 592-41-6, 1-Hexene; CAS No. 111-66-0, 1-Octene; CAS No. 872-05-9, 1-Decene; CAS No. 1120-36-1, 1-Tetradecene (Analytical Grade)

##### Method

**Method:** Acute static bioassay  
**GLP:** No

Type: Aquatic  
Species: Thirteen marine bacteria  
Exposure Period: 16 hours  
Analytical Monitoring: No data

**Test Conditions:** Water samples collected from Cleveland and Victoria Point on the Brisbane coast, southeastern Queensland, Australia, were cultured on marine salts medium solidified with 1.5% agar. Thirteen different marine bacteria were isolated and transferred to new media. This culture was maintained at 30°C and subcultured weekly. The test articles were dissolved in ethanol and added to media (maximum 0.1 ml in 50 ml). 0.1 mg of bacterial culture containing  $8 \times 10^{10}$  bacteria per ml was added. Each experiment was performed in triplicate. Controls consisting of bacteria inoculated into the medium, without test compounds, both with and without ethanol were run simultaneously. Absorbance at 600 nm was determined, followed by incubation without shaking at 30°C. After 16 hours, the absorbance was remeasured and the differences were calculated and expressed as a percentage of the difference in absorbance of the control. These data were then converted to Probit units and least-squares linear regression equation against toxicant concentration was obtained. From these regression equations, the effective concentration of the test compound that inhibits bacterial growth by 50 and /or 10% (EC50 and EC10, respectively) was determined.

**Results:** Only 1-hexene exerted a toxic effect [ $\log EC_{10} = -0.49$ ]; however, the calculated  $\log EC_{50}$  was 0.46, indicating a value >100% saturation in sea water. The other 1-alkenes were not toxic up to levels of 100% saturation.

**Reliability:** (1) Reliable without restrictions

**Reference:** Warne, M. St. J. Connell, D.W., Hawker, D. W., and G. Schuurmann (1989) Quantitative Structure-Activity Relationships for the Toxicity of Selected Shale Oil Components to Mixed Marine Bacteria. *Ecotoxicology and Environmental Safety*, 17: 133-148.

**Other:** This study was included in the dossiers for 1-hexene, 1-octene, and 1-tetradecene at SIAM 11. Additional information has been added.

### C. Test Substance

Identity: CAS No. 1120-36-1, 1-Tetradecene (practical grade)

#### Method

Method: No data  
GLP: No data  
Species: *Candida sp.* and *Saccharomyces calrsbergensis*  
Exposure Period: 1 or 3 days

<b>Analytical Monitoring:</b>	No
<b>Test Conditions:</b>	<p>Two species of <i>Candida</i> which can use n-alkanes above C8 for growth (<i>C. tropicalis</i> NCYC4 and <i>C. 107</i>), and <i>Saccharomyces carlsbergensis</i> (NCYC 530), which cannot grow on hydrocarbons, were used in this study. Organisms were grown in conical flasks at 30 °C with shaking. For testing, yeasts were collected by centrifugation, and washed with buffer before use.</p> <p>When tested with aliphatic compounds, glucose was at 25 g/L with 2.5 g malt extract/L of basal salts medium. This medium (20 mL) was in 100 mL flasks and inoculated with 0.1 mL of glucose-grown yeast. Alkanes and derivatives were tested at 10% (v/v). <i>Candida 107</i> was grown for one day, and the other yeast grown for 3 days. A Beckman laboratory oxygen analyzer was used for respiration measurements.</p>
<b>Results:</b>	<p>Good growth was seen in all three yeast tests with tetradecene and glucose. Good growth was seen with tetradecene alone in <i>Candida 107</i> and <i>C. tropicalis</i>. No growth was seen with <i>Saccharomyces carlsbergensis</i> and tetradecene in the absence of glucose.</p>
<b>Reliability:</b>	(1) Reliable without restrictions
<b>Reference:</b>	Gill, C.O., and Ratledge, C. (1972) Toxicity of n-Alkanes, n-Alk-1-enes, n-Alkan-1-bromides towards Yeasts. <i>Journal of General Microbiology</i> , 72:165-172.
<b>Other:</b>	This study was included in the dossier for 1-tetradecene at SIAM 11.

#### 4.5 Chronic Toxicity to Aquatic Organisms

No data available

#### 4.6 Toxicity to Terrestrial Organisms

##### A. Toxicity to Terrestrial Plants.

No data available

##### B. Toxicity to Soil Dwelling Organisms.

No data available

##### C. Toxicity to Other Non Mammalian Terrestrial Species (including Avian)

No data available

#### 4.7 Biological Effects Monitoring (including Biomagnification)

No data available

#### 4.8 Biotransformation and Kinetics

No data available

### 5. MAMMALIAN TOXICITY

#### 5.1 Toxicokinetics, Metabolism and Distribution

**Test Substance:** CAS No. 629-73-2, 1-Hexadecene

**Method** Non-standard  
**Test Type** in-vitro  
**GLP** No data available  
**Year** Unknown

**Method:** 1-Hexadecene and an epoxide hydrolase inhibitor were incubated with rabbit liver microsomes and an extract was analyzed.

**Test Conditions:** 1-Hexadecene (10  $\mu$ moles), dissolved in acetone, was incubated at 37°C for 30 min in air with rabbit liver microsomes (equivalent to 2 g tissue) suspended in 0.1 M phosphate buffer, pH 7.4, in the presence of a NADPH-generating system. The inhibitor, 1,2-epoxydecane (10 mM), was dissolved in the acetone together with the substrate. The reaction was terminated by the addition of 2ml 5N sodium hydroxide, and the mixture extracted with 30 ml ether containing 1,2-epoxytetradecane or 1,2-dihydroxytetradecane as the internal reference for the quantitative determination of metabolites. After concentration of the extract, the residual solution was subjected to silica gel thin-layer chromatography developed in benzene-acetone (5:1). Elution of epoxides and glycols from chromatograms was carried out separately with ethanol. The eluates were analyzed by gas-chromatography-mass spectroscopy.

**Results:** The formation of the epoxide (1,2-epoxyhexadecane, 2.4  $\mu$ g) was observed only when the olefin was incubated in the presence of the epoxide hydrolase inhibitor 1,2-epoxydecane. In the absence of inhibitor, 1,2-dihydroxyhexadecane was formed (16.1  $\mu$ g).

**Conclusions:** The authors concluded these results indicate that 1-hexadecene is metabolized to 1,2-dihydroxyhexadecane via 1,2-epoxyhexadecane.

**Reliability:** (1) Reliable without restrictions

**Reference:** Watabe, T. and Yamada, N. (1975) The biotransformation of 1-hexadecene to carcinogenic 1,2-epoxyhexadecane by hepatic microsomes. *Biochemical Pharmacology* 24 :1051-1053.

## 5.2 Acute Toxicity

### A. Acute oral toxicity

#### (1) Test Substance

Identity (purity): CAS No. 629-73-2, 1-Hexadecene (~93%, GULFTENE 16)

#### Method

Method/guideline: OECD 401  
Type (*test type*): LD50  
GLP: Yes  
Year: 1992  
Species/Strain: Sprague-Dawley Rat  
Sex: Male and female  
No. of animals per sex per dose: 5  
Vehicle: None  
Route of administration: Oral gavage

**Test Conditions:** The purpose of this peroral toxicity test was to assess the potential for neurotoxicity. The test material was administered as single gavage doses (5.0 g/kg) or divided gavage doses (10.0 g/kg) for which 2 equal portions were given approximately 1 hour apart to groups of 5 female and 5 male fasted Sprague-Dawley rats (weighing between 200 and 299 g, approximately 7-13 weeks of age). Following dosing, the animals were observed for 14 days. When clinical signs indicated neurotoxicity, a battery of functional tests was conducted on Days 1, 2, and 14, and additionally when thought necessary by the neurotoxicologist. Body weights were recorded on Days 0, 7, 14 and at termination. All animals were necropsied after death or sacrifice. Statistical methods were not specified.

#### Results:

Value: LD50 > 10,000 mg/kg  
Number of deaths at each dose level: No deaths were observed at 5.0 g/kg. At 10.0 g/kg, 2 of 5 males and 2 of 5 females died.

Remarks: At 10 g/kg, all animals showed signs of toxicity including wetness on perineal fur, red crust on perinasal and periocular fur,

greasy-textured fur, irritation and alopecia of extremities and abdominal area, red extremities, aggressive behavior (probably attributable to the local irritation), sluggishness, and excess discharge from the perineal area; 3/5 males and 3/5 females appeared to be emaciated; 1/5 males and 3/5 females exhibited kyphosis; 4/5 males and 5/5 females exhibited abnormal gait/hindlimb motion and/or walking on toes (probably resulting from the irritation). Several animals exhibited weight depression (or loss) through 7 days or more (mean weight change at 7 days: -43 g to 2 g [males] and -63 g to 1 g [females]; at 14 days: 7 g to 40 g [males] and -24 g to 32 g [females]). Necropsy (rats that died) revealed discoloration of lungs (1/2 males and females), intestines (2/2 males and females), liver (1/2 males) and kidneys (1/2 males). Survivors had no remarkable gross lesions.

At 5 g/kg, all animals showed signs of toxicity including greasy wetness on perineal fur and extending over the entire hindquarter area, red crust on perinasal fur, irritation and alopecia of perineal area and outer hindlimbs; 1/5 males and 5/5 females exhibited kyphosis; 1/5 males and 4/5 females were observed walking on toes (probably resulting from the irritation). All animals gained weight and had no remarkable gross lesions.

At both dose levels, microscopic evaluation of brains, spinal cords, sciatic nerves and pituitaries revealed no lesions.

A detailed neurotoxicological examination, showed numerous gait, postural and behavioral effects. Alterations in behavior were observed for all animals at 10 g/kg beginning 1 day after dosing. These were generally gone by the evaluation 14 days after dosing. The peak effects, with respect to number and severity of signs, were generally observed 2 days after dosing. Similar alterations, although less severe, were observed for animals treated with 5 g/kg during the first two days after treatment. These findings were considered likely to be secondary to irritation of the abdominal, perianal, and hindlimb areas caused by the excreted test material. This conclusion is based on the pattern of behavioral findings, the time course for the behavioral changes, clinical signs of irritation, and the lack of neuropathological lesions in the central or peripheral nervous system to support a conclusion of a primary neurotoxicant effect.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint.

**References:** Bushy Run Research Center (1992) GULFTENE 16 (Hexadecene-1): Acute peroral toxicity testing in the rat, Project 91N0035. Conducted for Chevron Research and Technology Company (unpublished report).

**(2) Test Substance**

Identity (purity): CAS No. 26952-14-7 (Hexadecene, >98%, 20-30% branched, double bond randomized along carbon chain)

**Method**

Method/guideline: EPA OPP 81-1  
Type (*test type*): LD50  
GLP: Yes [X] No [ ]  
Year: 1993  
Species/Strain: Rat/HSD:SD  
Sex: Males and females  
No. of animals per sex per dose: 5

Vehicle: None  
Route of administration: Oral gavage

**Test Conditions:** Single doses of 5050 mg/kg of undiluted test material were administered intragastrically to groups of 5 male and 5 female fasted albino rats (young adults, 208-238 g [males], 194-203 g [females]). Animals were observed for 14 days. Individual body weights were recorded on Days 0, 7, and 14. A gross necropsy was performed on each animal at the termination of the study. Statistical methods were not used.

**Results:**

Value: LD50 > 5050 mg/kg  
Number of deaths at each dose level: No deaths at 5050 mg/kg

Remarks: No deaths were observed. All animals gained weight during the study. Signs of toxicity included activity decrease in all females; and piloerection and polyuria seen in all animals, which were no longer evident by Day 7. Alopecia was observed in all animals on Days 7 through 14. The gross necropsy conducted on all animals at termination of the study revealed no observable abnormalities in any of the animals. The acute oral LD50 was greater than 5050 mg/kg.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Stillmeadow, Inc. (1993) C16 Alpha Olefin, Isomerized: Acute Oral Toxicity Study in Rats, Study No. 0490-93. Conducted for Chevron Chemical Company (unpublished report).

**(3) Test Substance**

Identity (purity): C10-14 Alpha Olefins

Remarks: Blend of CAS No. 872-05-9, 1-Decene; CAS No. 112-41-4, 1-Dodecene; CAS No. 1120-36-1, 1-Tetradecene (proportions unknown). Test substance was an olefins fraction distilled at 180E-240E containing 75% monoolefin.

**Method**

Method/guideline: no data  
Type (*test type*): LD50  
GLP: No  
Year: 1977  
Species/Strain: Rat and mouse  
Sex: no data  
No. of animals per sex per dose: no data

Vehicle: no data  
Route of administration: Oral gavage

**Test Conditions:** no data

**Results:**

Value: LD50 = 17.3 g/kg (mouse) and 21.3 g/kg (rat)

**Reliability:** (4) Not assignable

**References:** Abasov, D.M. Saffarova, I.A., Zeinalova, Kh.G. (1977) Toxicological characteristics of some alpha-olefins. Sb. Nauch. Tr. Nii. Gig. Trud. Prof. Zabol. 11:149-154.

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

**(4) Test Substance**

Identity (purity): C12-14 Alpha Olefins

Remarks: Blend of CAS No. 112-41-4, 1-Dodecene; CAS No. 1120-36-1, 1-Tetradecene (proportions unknown)

**Method**

Method/guideline: no data  
Type (*test type*): LD50  
GLP: No

Year: 1977  
Species/Strain: Rat  
Sex: no data  
No. of animals per sex per dose: no data  
Vehicle: no data  
Route of administration: Oral gavage  
**Test Conditions:** After a fast of 18 hours, a single oral dose of 10 g/kg body weight was given. Survival was such that the LD50 value was greater than 10 g/kg.

**Results:**

Value: LD50 > 10 g/kg

**Reliability:** (2) Reliable with restrictions: Incomplete reporting.

**References:** Ethyl Corporation (1977) Toxicology Evaluation of Ethyl Compound. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

(5) **Test Substance**

Identity (purity): C14-16 Alpha Olefins

Remarks: Blend of CAS No. 1120-36-1, 1-Tetradecene; CAS No. 629-73-2, 1-Hexadecene (proportions unknown)

**Method**

Method/guideline: no data  
Type (*test type*): LD50  
GLP: No  
Year: 1977  
Species/Strain: Rat  
Sex: no data  
No. of animals per sex per dose: no data  
Vehicle: no data  
Route of administration: Oral gavage

**Test Conditions:** After a fast of 18 hours, a single oral dose of 10 g/kg body weight was given. Survival was such that the LD50 value was greater than 10 g/kg.

**Results:**

Value: LD50 > 10 g/kg

**Reliability:** (2) Reliable with restrictions: Incomplete reporting.

**References:** Ethyl Corporation (1977) Toxicology Evaluation of Ethyl Compound. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

**B. Acute inhalation toxicity**

**(1) Test Substance**

Identity (purity): CAS No. 629-73-2, 1-Hexadecene (~93%)

**Method**

Method/guideline: 1-hr exposures to seven different concentrations in a dynamic exposure system.

Type (*test type*): LC50

GLP: Yes [ ] No [X ]

Year: 1967

Species/Strain: Rat/Wistar

Sex: Males

No. of animals per sex per dose: Not reported

Vehicle: None

Route of administration: Inhalation

**Test Conditions:** Groups of male albino Wistar rats weighing between 209 and 299 g were exposed for 1 hour to saturated mists of the test substance and observed for 14 days. The number of animals per group was not reported. The animals were observed for toxic signs during exposure and were periodically weighed for 14 days after exposure. On the 14th day, they were sacrificed for the determination of gross pathological changes.

The saturated mists were prepared by placing a Dautrabanda nebulizer within the exposure chamber and passing an air line and olefin feed line to it from outside. This aerosol generator produces particles no larger than 8  $\mu$  in diameter. It was found

experimentally that the maximum mist concentration was achieved when the nebulizer was operating at an air flow of 2 L/min with about 50 ml of olefin in the reservoir. Estimates of mist concentration were made from measurement of the volume loss from the nebulizer reservoir and total air flow through the system. Additionally, a sample holder containing a millipore filter was positioned downward in the chamber and air drawn through at a rate calculated to collect suspended particles of 2  $\mu$  or less. The lower size limit of collection by the filter was expected to be 0.45 $\mu$ . Papers were weighed before and after collection and the weight gain used to calculate concentration of particles in the 0.45-2.0  $\mu$  range. Statistical methods were not used.

**Results:**

Value: LC50 >8500 mg/m<sup>3</sup> (926 ppm)

Number of deaths  
at each dose level: None

Remarks: The aerosol generator produced particles that were <8 microns in diameter. Rats showed a drowsy appearance on removal from the chamber. The drowsiness/ lethargy disappeared rapidly when animals were removed from exposure. The fur of animals was "oily" from deposition of particles. There was no mortality and no significant weight change or gross pathological change on autopsy. Estimated exposure concentrations were 8500 mg/m<sup>3</sup> for particles <8 $\mu$  and 150 mg/m<sup>3</sup> for particles 0.45 - 2.0 $\mu$ . These concentrations represented very heavy mists. Visibility through the chamber (12" diameter) was impossible. The LC50 was > 8500 mg/m<sup>3</sup>.

**Reliability:** (2) Reliable with restrictions: No information is given on the number of animals dosed and there are limited details of procedures.

**Flag:** Key study for SIDS endpoint.

**References:** Rinehart, W.E. (1967) Toxicological Studies on Several Alpha Olefins. University of Pittsburgh, submitted to Gulf Research and Development Co. (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 629-73-2, 1-Hexadecene (min. 90.6% with vinylidenes [max. 7.5%], internal olefins [max. 2%], paraffins [max.1.5%] as impurities.

**Method**

**Method/guideline:** The test was performed in accordance with the OECD Guideline No. 403 "Acute Inhalation Toxicity", Adopted 12 May 1981 with only minor deviation in the measurement of humidity.

**Type (test type):** LC50  
**GLP:** Yes [ ] No [X ]  
**Year:** 1991  
**Species/Strain:** Rat/Wistar  
**Sex:** Males and females  
**No. of animals per sex per dose:** 5

**Vehicle:** None  
**Route of administration:** Inhalation (aerosol)

**Test Conditions:** The animals were received from breeding station VELAZ, Prague, Czech Republic. The rats were housed in a conventional animal house with artificial light-dark cycle (12h and 12h) in plastic cages. Microclimatic parameters :  $22 \pm 2$  °C, humidity 30-70 %. The rats were fed by standard pelleted diet (VELAZ, Prague) and tap water (quality for human consumption). Eight groups of 10 rats each (5 males and 5 females, weight 161-266 g) were exposed for 4 hrs to concentrations of 0, 2.37, 3.29, 4.00, 4.88, 5.75, 6.64, and 7.68 mg/L (0, 258, 358, 436, 532, 626, 723, 836 ppm). The test substance was administered in air using a glass, nose-only inhalation chamber with a flow rate of 0.66 m<sup>3</sup>/hr. The air flow was maintained to allow 12-15 changes of air per hour. Slight negative pressure was maintained in the chamber during the test. Air flow was measured continually. The temperature, but not humidity, was measured inside the apparatus. The test substance was delivered to the chamber by an aerosol generator. Actual concentration of the test substance in the test chamber was measured gravimetrically in 30 min intervals. The particle size was also measured. The mean value was 4.78 µm.

After the exposure, the rats were moved to separate cages. Times of deaths were recorded precisely. Rats that died during exposure were immediately necropsied and samples were taken for histopathology evaluation. During the 14 days following exposure, rats were observed twice per day with a 4-hr interval between observations. At the end of the 14-day observation period, the animals were euthanized and necropsied, and samples were taken for histopathology evaluation. Rats were weighed after exposure and on Day 7 and Day 14.

**Results:**

Value: LC50: 6.359 g/m<sup>3</sup> (6.359 mg/L, 693 ppm)  
 Number of deaths at each dose level: See Remarks

Concentration (mg/l)	Occurrence of pathological signs (M/FM)	Num. of deaths (M/FM)	Time of death (min)
2.37	10 (5/5)	0	
3.29	10 (5/5)	2 (2/0)	76M,182FM
4.00	10 (5/5)	2 (1/1)	45FM, at 16hrs M
4.88	10 (5/5)	2 (2/0)	43M,50FM
5.75	10 (5/5)	4 (2/2)	78FM,195FM,5 after finish of appl., at 16hrsM
6.64	10 (5/5)	4 (3/1)	45M,143M, at16hrs M+FM
7.68	10 (5/5)	8 (4/4)	48FM, 59M+FM, 70M+FM, 192M, until 16hrs M+FM

Effects were not dose-dependent. The only concentration without signs of toxic effects at 24 hrs after exposure was 2.37 g/m<sup>3</sup>. Exposure of rats to higher concentrations caused only slight eye-lid turgidity connected with mild flux from nose and eyes. Microscopic changes that could be associated with exposure to the test substance were seen in the respiratory tract at 3.29 g/m<sup>3</sup> and above. These changes observed in the lung were suggestive of lung congestion and acute hypertension accompanied by hemorrhage. No histopathology was found in animals that survived to the end of the study (14 days).

**Conclusions:** The LC50 = 6.359 (5.502-7.337) g/m<sup>3</sup>, determined by Bliss method. 1-hexadecene at  $\geq 3.29$  g/m<sup>3</sup> caused acute hypertension accompanied by hemorrhage in the lungs. (conclusions of study author)

**Reliability:** (2) Reliable with restrictions; the study was not conducted under GLPs

**References:** Research Institute of Organic Synthesis a.s (1991) Pardubice, Czech Republic, Test No. T2219 (unpublished report).

(3) **Test Substance**

Identity (purity): C10-14 Alpha Olefins

Remarks: Blend of CAS No. 872-05-9, 1-Decene; CAS No. 112-41-4, 1-Dodecene; CAS No. 1120-36-1, 1-Tetradecene (proportions unknown). Test substance was an olefins fraction distilled at 180E-240E containing 75% monoolefin.

**Method**

Method/guideline: no data  
Type (*test type*): LC50  
GLP: No  
Year: 1977  
Species/Strain: mouse  
Sex: no data  
No. of animals per sex per dose: no data  
Vehicle: no data  
Route of administration: inhalation

**Test Conditions:** no data

**Results:**

Value: LC50 = 223 mg/L

**Reliability:** (4) Not assignable

**References:** Abasov, D.M. Saffarova, I.A., Zeinalova, Kh.G. (1977)  
Toxicological characteristics of some alpha-olefins. Sb. Nauch. Tr. Nii. Gig. Trud. Prof. Zabol. 11:149-154.

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

(4) **Test Substance**

Identity (purity): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

**Method**

Method/guideline: 1-hr exposures to seven different concentrations in a dynamic exposure system.  
Type (*test type*): LC50  
GLP: Yes [ ] No [X]  
Year: 1967  
Species/Strain: Rat/Wistar  
Sex: Males  
No. of animals per sex per dose: Not reported

**Vehicle:** None

**Route of administration:** Inhalation

**Test Conditions:** Groups of male albino Wistar rats weighing between 209 and 299 g were exposed for 1 hour to saturated mists of the test substance and observed for 14 days. The number of animals per group was not reported. The animals were observed for toxic signs during exposure and were periodically weighed for 14 days after exposure. On the 14th day, they were sacrificed for the determination of gross pathological changes.

The saturated mists were prepared by placing a Dautrabanda nebulizer within the exposure chamber and passing an air line and olefin feed line to it from outside. This aerosol generator produces particles no larger than 8  $\mu$  in diameter. It was found experimentally that the maximum mist concentration was achieved when the nebulizer was operating at an air flow of 2 L/min with about 50 ml of olefin in the reservoir. Estimates of mist concentration were made from measurement of the volume loss from the nebulizer reservoir and total air flow through the system. Additionally, a sample holder containing a millipore filter was positioned downward in the chamber and air drawn through at a rate calculated to collect suspended particles of 2  $\mu$  or less. The lower size limit of collection by the filter was expected to be 0.45 $\mu$ . Papers were weighed before and after collection and the weight gain used to calculate concentration of particles in the 0.45-2.0  $\mu$  range. Statistical methods were not used.

**Results:**

**Value:** LC50 >9900 mg/m<sup>3</sup> (1438 ppm)

**Number of deaths at each dose level:** None

**Remarks:** The aerosol generator produced particles that were <8 microns in diameter. Rats showed a drowsy appearance on removal from the chamber. The drowsiness/ lethargy disappeared rapidly when animals were removed from exposure. The fur of animals was "oily" from deposition of particles. There was no mortality and no significant weight change or gross pathological change on autopsy. Estimated exposure concentrations were 9900 mg/m<sup>3</sup> for particles <8 $\mu$  and 100 mg/m<sup>3</sup> for particles 0.45 - 2.0 $\mu$ . These concentrations represented very heavy mists. Visibility through the chamber (12" diameter) was impossible. The LC50 was > 9900 mg/m<sup>3</sup>.

**Reliability:** (2) Reliable with restrictions: No information is given on the number of animals dosed and there are limited details of procedures.

**References:** Rinehart, W.E. (1967) Toxicological Studies on Several Alpha Olefins. University of Pittsburgh, submitted to Gulf Research and Development Co. (unpublished report).

**Other:** This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

### C. Acute dermal toxicity

#### (1) Test Substance

**Identity (purity):** CAS No. 68855-59-4, C14-16 Alpha Olefin Blend (Typical composition C12-1.3%, C14-64.7%, C16-33%, C18-1%, mono-olefin 99.6%, linear terminal 76%, branched terminal 19%, linear internal 5%)

#### Method

**Method/guideline:** Not specified  
**Type (test type):** LD50  
**GLP:** No  
**Year:** 1976  
**Species/Strain:** Rabbits/New Zealand White  
**Sex:** Males and females  
**No. of animals per sex per dose:** 2 males, 2 females  
**Vehicle:** None  
**Route of administration:** Dermal

**Test Conditions:** A C14-16 alpha olefin blend was tested for single dose dermal toxicity in rabbits. Four New Zealand white rabbits (2 male and 2 female, 2.3-3.0 kg) were used. A dose of 10 grams per kilogram body weight was applied to clipped and abraded test sites. Sites were occluded for 24 hours and animals observed for 14 days.

#### Results:

**Value:** LD50 > 10 g/kg  
**Number of deaths at each dose level:** No rabbits died during the 14-day observation period and there were no visible signs of toxicity. There was slight erythema on the first day of observation.

**Remarks:** Survival was such that LD50's were stated to be greater than 10 grams per kilogram body weight.

**Reliability:** (2) Reliable with restrictions: incomplete reporting

**Flag:** Key study for SIDS endpoint

**Reference:** Carte, G. *A report on the Acute Toxicity of Alpha Olefins C14-16*  
Tulane University School of Medicine August 1976; Ethyl Corporation, Sponsor (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

(2) **Test Substance**

**Identity (purity):** CAS No. 26952-14-7, Hexadecene (>98%)

**Method**

**Method/guideline:** EPA OPP 81-2  
**Type (test type):** LD50  
**GLP:** Yes  
**Year:** 1993  
**Species/Strain:** Rabbit/New Zealand white  
**Sex:** Males and females  
**No. of animals per sex per dose:** 5

**Vehicle:** None  
**Route of administration:** Dermal

**Test Conditions:** The objective of this study was to determine the acute dermal toxicity potential of the test material. Each animal was prepared on the day prior to treatment by clipping the dorsal surface of the trunk free of hair to expose not less than 10% of the total body surface area. Five albino rabbits of each sex (young adult [3-6 mos] weighing 2.425-2.875 kg [males] and 2.400-2.750 kg [females] were treated with a single dermal application of 2020 mg/kg of undiluted test material for 24 hours. The treated area was covered with gauze and a semi-permeable dressing (orthopedic stockinette) to retard evaporation of volatile substances and to prevent possible ingestion of the test material. After 24 hours the wrappings and gauze were removed from the animals. The exposed areas were gently washed with room temperature tap water and a clean wet cloth was used to remove as much remaining test material as possible. Animals were observed for pharmacologic and/or toxicologic signs including signs of dermal irritation frequently throughout the study.

Individual body weights were recorded on Days 0, 7, and 14. A gross necropsy was conducted on each animal at the termination of the study. Statistical methods were not used.

**Results:**

**Value:** LD50 > 2020 mg/kg  
**Number of deaths at each dose level:** One male died on Day 14 after final observations had been made, but it was not considered to be test material related.

**Remarks:** All surviving animals appeared normal for the duration of the study and gained weight. The gross necropsy conducted on each animal at termination of the study revealed no observable abnormalities in any of the animals. The acute dermal LD50 was greater than 2020 mg/kg.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Stillmeadow, Inc. (1993) Acute Dermal Toxicity Study in Rabbits, Study No. 0491-93. Conducted for Chevron Chemical Company (unpublished report).

(3) **Test Substance**

**Identity (purity):** C12-14 Alpha Olefin Blend

**Remarks:** Blend of CAS No. 112-41-4, 1-Dodecene; CAS No. 1120-36-1, 1-Tetradecene

**Method**

**Method/guideline:** Not specified  
**Type (test type):** LD50  
**GLP:** No  
**Year:** 1976  
**Species/Strain:** Rabbits/New Zealand White  
**Sex:** Males and females  
**No. of animals per sex per dose:** no data

**Vehicle:** None  
**Route of administration:** Dermal

**Test Conditions:** A C12-14 alpha olefin blend was tested for single dose dermal toxicity in rabbits. Six New Zealand white rabbits were used. A dose of 10 grams per kilogram body weight was applied to

clipped and abraded test sites. Sites were occluded for 24 hours and animals observed for 14 days.

**Results:**

Value: LD50 > 10 g/kg

Number of deaths  
at each dose level: no data

Remarks: Survival was such that LD50's were stated to be greater than 10 grams per kilogram body weight.

**Reliability:** (2) Reliable with restrictions: incomplete reporting

**Reference:** Ethyl Corporation (1977) Toxicology Evaluation of Ethyl Compound. Gulf South Research Institute P.O. Box 1177 New Iberia, LA 70560 (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

**D. Acute toxicity, other routes**

No data available

**5.3 Corrosiveness/Irritation**

**A. Skin Irritation/Corrosion**

(1) **Test Substance:** CAS No. 629-73-2, 1-Hexadecene (~93%, GULFTENE 16)

pH: Not applicable

**Method:** OECD 404

Test Type: in vivo

GLP: Yes

Year: 1995

**Test Conditions**

Species: Rabbits

Strain: New Zealand White

Cell type:

Sex: Male and female

Number of animals  
per sex per dose: 5 males and 1 female

Total dose: 0.5 ml  
Vehicle: None  
Exposure time period: 4 hrs  
Grading scale: Draize

**Method Remarks:** At the start of the study, the animals weighed 2.44 to 2.62 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabraded skin on the shaved backs of 6 rabbits, under a semi-occluded dressing (cotton gauze patch placed in position with a strip of porous tape; trunk wrapped in an elasticated corset [TUBIGRIP]). A contralateral area of untreated skin was identified to serve as the control against which the reactions of the treated site were evaluated. Four hours after application, the corset and patches were removed and residual test material was removed by swabbing with cotton wool soaked in 74% Industrial Methylated Spirits. The control sites were similarly swabbed. Scores were made for erythema and edema at 0.5, 24, 48, 72 and 96 hr after removal of patches, and at 7 and 14 days after initiation of exposure.

**Results:** The 4-hr exposure produced very slight erythema at two treated skin sites with well-defined erythema at 4 treated skin sites at the 30-minute observation. Very slight erythema was noted at one treated skin site and well-defined erythema at 5 treated sites at the 24-hr observation. Very slight erythema was apparent at all treated skin sites at the 48 and 72-hr observations and persisted at 5 treated skin sites at the 96-hr observation. Desquamation was noted at 5 treated sites at the 72-hr observation and at all treated sites at the 96-hr, 7 and 14-day observations. The desquamation apparent at the 14-day observation was considered to be reversible. The dermal reactions extended up to 4 cm beyond all treated skin sites during the study. Very slight edema was noted at 2 treated sites and slight edema at 4 treated skin sites at the 30-minute and 24-hr observations. Very slight edema was noted at 4 treated sites at the 48-hr observation and persisted at 2 sites at the 72-hr observation. The Draize primary irritation index was 2.46. The mean 24-72 hr scores for erythema and edema were 1.3 and 0.9, respectively.

**Reliability:** (1) Reliable without restrictions

**Reference:** Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 16, Report 703/076. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

(2) **Test Substance:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

pH: Not applicable

**Method:** OECD 404 except that only 3 animals were employed

Test Type: in vivo

GLP: Yes

Year: 1994

**Test Conditions**

Species: Rabbits

Strain: New Zealand White

Cell type:

Sex: Male and female

Number of animals per sex per dose: 2 males and 1 female

Total dose: 0.5 ml

Vehicle: None

Exposure time period: 4 hr

Grading scale: Draize

**Method Remarks:** At the start of the study, the animals (young adults) weighed 2.0 to 3.5 kg. One-half ml undiluted material was applied to the unabraded skin (approximately 6.25 cm<sup>2</sup>) on the shaved backs of 3 rabbits, under a semi-occluded dressing (cotton gauze patch covered with porous tape; trunk loosely wrapped with a sheet of Texwipe® cotton cloth). Each rabbit was fitted with an Elizabethan collar during the exposure period. A contralateral area of untreated skin served as the control against which reactions of the treated site were evaluated. After 4 hrs, patches were removed and residual test substance was removed using a paper towel moistened with tap water. Scores were made for erythema and edema at 1, 24, 48 and 72 hr, and at 7 and 14 days after initiation of exposure.

**Results:** The 4-hr exposure produced well-defined erythema and very slight to slight edema which cleared by day 14. No physical or behavioral abnormalities were observed in any animal. The Draize primary irritation index was 2.2/8. The averages (for each animal) of 24-72 scores were 1.3, 2.0, and 1.3 for erythema and 0.0, 0.3, and 0.3 for edema.

**Reliability:** (1) Reliable without restrictions

**Reference:** Morris, T. (1995) Acute dermal irritation screening study in rabbits with C16/C18 Alpha Olefins, Isomerized. Conducted by Hill Top Biolabs, Inc., Project No. 94-8345-21 (A), for Chevron Research and Technology Company (unpublished report).

**(3) Test Substance**

Identity (purity): CAS No. 629-73-2, 1-Hexadecene

**Method**

Method/guideline:

Test type: Repeated irritation  
GLP: No  
Year: 1963  
Species: Guinea pig  
Strain: No data  
Route of Administration: Dermal  
Duration of test: 20 days  
Doses: 0.5 – 0.6 ml/day  
Sex: Males and/or females  
Exposure period: 7 days  
Frequency of treatment: 4 alternate days

Control group and treatment: Untreated control group

Post exposure observation period: 20 days following first treatment

Statistical methods: None

**Test Conditions:**

On the first day of the experiment, the hair from each side of 2 or 3 albino guinea pigs (300-500 g) was clipped. The test article was applied with a small atomizer to the left side of the animal and the right side was left untreated. Topical applications were made on days 1, 3, 5 and 7. The report did not indicate that the treated sites were covered or cleaned between or after applications. Subjective evaluations of skin irritancy were made every other day for 20 days following the first treatment. The skin characteristics grossly evaluated, each on a scale of 1-5, were: (1) erythema, (2) thickening, (3) hyperkeratinization, (4) desquamation or scaling and (5) formation of fissures and open lesions. From the total ratings for the 5 characteristics through the 20-day period, relative overall skin ratings from 0-8 were given.

**Results:** Irritating

**Remarks:** 1-Hexadecene was severely irritating with a maximum score of 8.

**Reliability:** (2) Reliable with restrictions: Not a guideline study and not conducted under GLPs. Incomplete reporting of details.

**References:** Hoekstra, W.G., and P.H. Phillips (1963) Effects of topically applied mineral oil fractions on the skin of guinea pigs. *J. Invest. Derm.* 40(2):79-88.

(4) **Test Substance:** CAS No. 1120-36-1, 1-Tetradecene

**pH:** Not applicable

**Method:** OECD 404

**Test Type:** in vivo

**GLP:** Yes

**Year:** 1995

**Test Conditions**

**Species:** Rabbits

**Strain:** New Zealand White

**Cell type:**

**Sex:** Male and female

**Number of animals per sex per dose:** 5 males and 1 female

**Total dose:** 0.5 ml

**Vehicle:** None

**Exposure time period:** 4 hrs

**Grading scale:** Draize

**Method Remarks:** At the start of the study, the animals weighed 2.37 to 2.69 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabraded skin on the shaved backs of 6 rabbits, under a semi-occluded dressing (cotton gauze patch placed in position with a strip of porous tape; trunk wrapped in an elasticated corset [TUBIGRIP]). A contralateral area of untreated skin was identified to serve as the control against which the reactions of the treated site were evaluated. Four hours after application, the corset and patches were removed and residual test material was removed by swabbing with cotton wool soaked in 74% Industrial Methylated Spirits. The control sites were similarly swabbed. Scores were made for erythema and edema at 0.5, 24, 48, 72 and 96 hr after removal of patches, and at 7 and 14 days after initiation of exposure.

**Results:** The 4-hr exposure produced well-defined erythema at five treated skin sites with very slight erythema at 1 treated skin sites at the 30-minute observation. Well-defined erythema was noted at all treated sites at the 24-hr observation. Very slight erythema was apparent at all treated skin sites at the 48 and 72-hr observations and at 5 treated skin sites at the 96-hr observation. Desquamation was noted at 1 treated site at the 72-hr observation and at all treated sites at the 96-hr, 7 and 14-day observations. The desquamation apparent at the 14-day observation was considered to be reversible. The dermal reactions extended up to 5 cm beyond each treated skin site during the study. Slight edema was noted at 5 treated sites and moderate edema at 1 treated skin site at the 30-minute observation. Slight edema was apparent at all treated skin sites at the 24-hr observation. Very slight edema was noted at all treated sites at the 48-hr observation and persisted at 1 site at the 72-hr observation. The Draize primary irritation index was 2.79. The mean 24-72 hr scores for erythema and edema were 1.3 and 1.1, respectively.

**Reliability:** (1) Reliable without restrictions

**Reference:** Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 14, Report 703/079. Conducted by Safepharma Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

## B. Eye Irritation/Corrosion

(1) **Test Substance:** CAS No. 629-73-2, 1-Hexadecene (~93%)

pH: Not applicable

**Method:** equivalent to OECD 405

Test Type: in vivo

GLP: No

Year: 1967

### Test Conditions

Species: Albino rabbits

Strain: Not specified

Cell type:

Sex: Males

Number of animals per dose: 6

Dose(s) used: 0.1 ml

Vehicle: None

Observation period: 72 hrs

Scoring method used: Draize scoring at 24, 48, and 72 hours after treatment

**Remarks:** A positive control group were exposed to 5% Ivory Soap solution

**Results:** Draize score at 24 hours was 1.3/110; it was 0.3 at 48 hours and 0.0 at 72 hours. The mean 24-72 hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis, respectively, were 0, 0, 0.3, and 0.

**Reliability:** (1) Reliable without restrictions

**Reference:** Rinehart, W.E. (1967) Toxicological Studies of Several Alpha Olefins Conducted by Department of Occupational Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania, for Gulf Research and Development Company (unpublished report).

(2) **Test Substance:** CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

**pH:** Not applicable

**Method:** OECD 405 except that only 3 animals were used

**Test Type:** in vivo  
**GLP:** Yes  
**Year:** 1994

**Test Conditions**

**Species:** Rabbits  
**Strain:** New Zealand White  
**Cell type:**  
**Sex:** Male and females  
**Number of animals per dose:** 1 male and 2 females

**Dose(s) used:** 0.1 ml  
**Vehicle:** None  
**Observation period:** 72 hrs  
**Scoring method used:** Draize scoring at 1, 24, 48, and 72 hours after treatment

**Remarks:** Young adult rabbits weighing 3.005 to 3.079 kg were used. The undiluted test substance was applied to one eye of each animal. The lids were gently held together for approximately one second. The eyes were rinsed after 24 hours. The eyes were examined for ocular irritation at 1, 24, 48 and 72 hrs following treatment. With the exception of the 1 hr scoring, all eyes were scored again for corneal opacity, intensity, and area using sodium fluorescein. Each

animal was also observed daily for any physiological or behavioral abnormalities.

**Results:** Draize score at 24 hours was 2.0/110 for eyes scored with and without sodium fluorescein. The average of the 24-72 hr scores for each animal were 0 for corneal opacity and iritis; 0.0, 0.33, and 0.33 for conjunctival redness, and 0.0, 0.33, and 0.0 for conjunctival chemosis.

**Remarks:** The test substance did not produce corneal opacity or iritis but did produce conjunctival irritation which was observed at the 1 and 24-hr readings. All eyes were clear at the 48-hr reading. The maximum total irritation score observed for individual animals was 4.

**Reliability:** (1) Reliable without restrictions

**Reference:** Morris, T. (1995) Acute eye irritation screening study in rabbits with C16/C18 Alpha Olefins, Isomerized. Conducted by Hill Top Biolabs, Inc., Project No. 94-8346-21 (A), for Chevron Chemical Company (unpublished report).

(3) **Test Substance:** C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

**Remark:** Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

**pH:** Not applicable

**Method:** equivalent to OECD 405

**Test Type:** in vivo

**GLP:** No

**Year:** 1967

#### **Test Conditions**

**Species:** Albino rabbits

**Strain:** Not specified

**Cell type:**

**Sex:** Males

**Number of animals per dose:** 6

**Dose(s) used:** 0.1 ml

**Vehicle:** None

**Observation period:** 72 hrs

Scoring method used: Draize scoring at 24, 48, and 72 hours after treatment

Remarks: A positive control group were exposed to 5% Ivory Soap solution

Results: Draize score at 24 hours was 1.0/110. It was 0.7 at 48 hours, and 1.3 at 72 hours. No scores greater than zero were seen in any animal for the cornea or iris at any time point. Maximum erythema scores were "1" in 3/6 animals at 24 hrs. Two animals had a score of "1" for erythema at 48 hrs. Four animals had "1" at 72 hrs. i.

Reliability: (1) Reliable without restrictions

Reference: Rinehart, W.E. (1967) Toxicological Studies of Several Alpha Olefins Conducted by Department of Occupational Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania, for Gulf Research and Development Company (unpublished report).

#### 5.4 Skin Sensitisation

A. **Test Substance:** CAS No. 629-73-2, 1-Hexadecene (NEODENE 16 Alpha Olefin)

**Method:** Buehler  
**Test Type:** challenge  
**GLP:** Yes  
**Year:** 1992

**Test Conditions**

**Species:** Guinea pig  
**Strain:** Hartley albino  
**Sex:** Male and female  
**Number of animals per sex per dose:** 4 each primary irritation, 10 each test group, 5 each control group

**Route of administration:** Topical

**Induction conc.:** 100%  
**Induction vehicle:** None  
**Challenge conc.:** 100%  
**Challenge vehicle:** Acetone  
**Grading system used:** Buehler

0=no reaction  
+/-= slight, patchy erythema  
1=slight but confluent, or moderate patchy erythema  
2=moderate erythema  
3=severe erythema with or without edema

Remarks:	Buehler, 1965; Ritz and Buehler, 1980
Method remarks:	<p>A Test Group of 10 male and 10 female animals, weighing 330 to 526 grams, was dosed topically at 0.5 ml/site under occlusion with test material once per week for three weeks, a total of three induction exposures. Doses were applied under 25-mm Hill Top Chambers®, with adhesive backs removed, occluded with plastic wrap and overwrapped with Elastoplast® tape. The period of exposure was six hours, after which the bandages were removed, and the sites wiped with disposable paper towels moistened with tepid tap water. The test material concentration used for induction and dosing (10% and 2.5% in acetone, respectively) were selected based on the irritation rangefinding phase. Two weeks after the last induction exposure, a challenge dose was given at the original site and a virgin site. A Naive Control Group (which had never before been exposed to the test material) of 5 males and 5 females was dosed with the test material at this time. Reactions to challenge dosing were evaluated at approximately 24 and 48 hours after completion of each exposure.</p> <p>Positive when 15 % of animals show a reaction at 24 and/or 48 H.</p>
<b>Results:</b>	Negative for sensitization
Grades:	All animals were +/-
Results Remarks:	Number of animals with skin reaction at challenge: 0/10 Number of animals with skin reaction in control group at challenge: 0/10.
<b>Reliability:</b>	(1) Reliable without restrictions
<b>Reference:</b>	<p>Morris, T. (1992) Delayed contact hypersensitivity study in guinea pigs (Buehler technique). Conducted by Hill Top Biolabs, Inc., Project No. 91-8382-21 (B), for Shell Oil Company (unpublished report).</p> <p>Buehler, E.V. (1965) Delayed contact hypersensitivity in the guinea pig, <i>Archives of Dermatology</i> 91:171-177.</p> <p>Ritz, H.L. and E.V. Buehler (1980) Planning, conduct and interpretation of guinea pig sensitization patch tests in <i>Current Concepts in Cutaneous Toxicity</i>, ed. V. Drill and P. Lazar. Academic Press, New York, N.Y. pp. 25-42.</p>
<b>B. Test Substance:</b>	CAS No. 26952-14-7 (Hexadecene, 49%) and 27070-58-2 (Octadecene 49%) with 2% C32-36 olefins as impurities; double bond occurs at all locations along the carbon chain; 20-30% methyl branching

**Method:** Buehler

Test Type: challenge

GLP: Yes

Year: 1994

### Test Conditions

Species: Albino guinea pig

Strain: Hartley

Sex: Males and females

Number of animals

per sex per dose: 1<sup>st</sup> Pilot (4 doses) = 1, 2<sup>nd</sup> Pilot (4 doses) = 1, Induction = 10, Challenge = 5, Rechallenge = 5

Route of administration: Topical

Induction conc.: 5% for test substance

Induction vehicle: Mineral Oil Light U.S.P. for test substance, 95% ethyl alcohol for positive control

Challenge conc.: 5% for test substance

Challenge vehicle: Mineral Oil Light U.S.P. for test substance, acetone for positive control

Grading system used: 0 = no reaction,  $\pm$  = slight, patchy erythema, 1 = slight but confluent, or moderate patchy erythema, 2 = moderate erythema, 3 = severe erythema with or without edema

Method remarks: At the start of the induction phase, the body weight range of the test and primary challenge animals ranged from 336-493 g; animals were the same age ( $\pm$  5 days) and were 6-11 weeks old. At the start of the rechallenge phase, the body weights of the rechallenge animals ranged from 426-599 g.

**HISTORICAL POSITIVE CONTROL GROUP:** 10 animals received 3 induction treatments with  $\alpha$ -hexylcinnamaldehyde (HC) (tech., 85%) at concentrations of 5% w/v in 95% ethanol. Approx. 2 wks following induction, a primary challenge treatment was conducted with the 10 test animals and 4 naïve control animals with HC at 5%, 2.5%, and 1.0% w/v in acetone. 13 days following primary challenge treatment, a rechallenge treatment was conducted with the 10 test animals and 5 naïve control animals with HC at 5% w/v in acetone.

**PILOT (IRRITATION SCREENING):** The irritation potential of the test material at levels of undiluted, 50%, 25%, 10%, 5%, 2.5%, 1%, and 0.5% were evaluated. The position of the different concentrations on the animals were varied to adjust for possible site-to-site variation in response. One day prior to exposure, hair was removed from backs with clippers. 0.3 ml test preparation was applied to a 25 mm Hill Top Chamber®. The animal was placed into a restrainer, the chamber was applied to the clipped surface, and the chamber was occluded with rubber

dental dam. Approximately 6 hr later, the chamber and restrainer were removed.

**INDUCTION:** An undiluted concentration of C16/C18 Alpha Olefins, Isomerized in Mineral Oil, was chosen for induction. The left shoulders of 20 animals were clipped the day before exposure. The clipped areas were exposed and animals restrained as described for the Pilot. The procedure was repeated at the same site once a week for 2 wks. After the last induction exposure, the animals were left untreated for 12 days.

**PRIMARY CHALLENGE:** Using the same procedure as in the induction phase but at a different skin site, the test animals (10 M, 9 F) were again exposed to the test material (5% in Mineral Oil). In addition, 10 naïve animals were treated with the test material.

**RECHALLENGE:** 7 days after primary challenge, test animals (10 M, 9 F) were again exposed to the test material (5% in Mineral Oil). In addition, 10 naïve animals were treated with the test material.

**OBSERVATIONS:** On the day following irritation screening, primary challenge, and rechallenge, animals were depilated and, 2 hr later, scored. Scoring was repeated the following day. No statistical analysis was conducted.

**Results:** Animals treated with C16/C18 Alpha Olefin, Isomerized were not sensitized

**Grades:** The incidence of grade 1 responses in the test group (12/19) compared to that of the naïve control group (4/10) suggested the possibility that sensitization might have been induced. Following rechallenge, the incidence of grade 1 responses in the test group (12/19) compared to that of the naïve control group (8/10) indicated that sensitization had not been induced.

**Results Remarks:** One female was found dead 3 days after first induction application. Cause of death was not determined.

**Reliability:** (1) Reliable without restrictions

**Reference:** Morris, T. (1995) Delayed contact hypersensitivity study in guinea pigs (Buehler technique). Conducted by Hill Top Biolabs, Inc., Project No. 94-8414-21, for Chevron Research and Technology Company (unpublished report).

**C. Test Substance:** C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

**Remarks** Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary

GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

**Method:** Landsteiner technique  
**Test Type:** challenge  
**GLP:** No  
**Year:** 1967

**Test Conditions**

**Species:** Albino guinea pig  
**Strain:**  
**Sex:** Males  
**Number of animals per sex per dose:** 10

**Route of administration:** Topical

**Induction conc.:** 100% for test substance  
**Induction vehicle:** None for test substance, 50% ethyl alcohol for positive control  
**Challenge conc.:** 100% for test substance  
**Challenge vehicle:** None for test substance, 50% ethyl alcohol for positive control  
**Grading system used:** Not specified

**Method remarks:** Three groups of ten male albino guinea pigs weighing 300-350 g each were used. A positive control group was exposed to 0.5% chlorodinitrobenzene in 50% ethyl alcohol in water. A second group was exposed to 50% ethyl alcohol only. The other group received olefin test article. Test sites on the backs of the animals were clipped and light abrasions of the outer dermal layer were made with a needle. 0.1 ml test article was applied to the test sites from a dropper and rubbed into the skin with a glass rod, three times weekly for nine applications. Type of dressing was not specified. Observations for erythema and edema were made 24 hours after applications. After the ninth application, animals were rested for two weeks. They were then challenged with 0.1 ml of test article or 0.5% chlorodinitrobenzene in 50% ethanol-water (the ethanol control animals also received chlorodinitrobenzene).

**Results:** Animals treated with C12-16 Alpha Olefin Fraction were not sensitized

**Grades:** See Remarks

**Remarks:** Only slight erythema was seen in one animal exposed to the alpha olefin after the eighth application and in two animals after the ninth application; no edema was seen. Animals exposed to alcohol showed no reactions at any time point. The positive control animals showed moderate erythema in all animals after the third application, and mild edema in half the animals after the seventh application. During the 2-wk rest interval, signs of erythema and edema disappeared from all animals.

Twenty-four hours after the challenge, alpha olefin treated animals showed no response. The positive control group showed severe erythema in all animals. The animals pre-treated with alcohol given chlorodinitrobenzene as a challenge for comparison with the positive control group showed only a very slight erythema in 2 animals.

**Reliability:** (1) Reliable without restrictions

**Reference:** Rinehart, W.E. (1967) Toxicological Studies of Several Alpha Olefins Conducted by Department of Occupational Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania, for Gulf Research and Development Company (unpublished report).

## 5.5 Repeated Dose Toxicity

### A. Test Substance

**Identity (purity):** C16/18 isomerised olefin  
**Remarks:** C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%. Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

### Method

**Method/guideline:** OECD 407  
**Test type:** subacute toxicity  
**GLP:** Yes  
**Year:** 2000  
**Species:** Rat  
**Strain:** Sprague Dawley (crl:CD BR)  
**Route of Administration:** Oral gavage  
**Duration of test:** 4 weeks  
**Doses:** 0, 25, 150, or 1000 mg/kg/day  
**Sex:** Males and females  
**Exposure period:** 4 weeks  
**Frequency of treatment:** Once daily, 7 days/week  
**Control group and treatment:** Concurrent vehicle control (corn oil)  
**Post exposure observation period:** None

**Statistical methods:** Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)

**Test Conditions:** Groups of ten rats (5M:5F) were dosed orally by gavage once daily over a period of 28 days. Animals were approximately 41 days old on the first day of dosing. Animals were regularly monitored for any signs of ill health or reaction to treatment. Detailed functional observations were performed weekly, with additional functional observations performed during pretrial and week four. Animals were weighed daily to determine dose. Body weights and food consumption were recorded twice weekly. Blood and urine samples were collected during week four of the study. After four weeks of treatment, animals were sacrificed and subjected to necropsy. A comprehensive list of organs were weighed and /or preserved (adrenal, brain, epididymis, eye, gastrointestinal tract including stomach, duodenum, jejunum, ileum, caecum, colon, rectum, heart, kidney, liver, lung, bone marrow, mesenteric lymph node, ovary, pituitary, prostate, sciatic nerve, spinal cord, spleen, submandibular lymph node, testis, thymus, thyroid with parathyroid, trachea, urinary bladder, uterus). Tissues from the controls and high dose animals were subjected to histological examination. Histology was also performed on the male kidneys from the lower doses.

## Results

**NOAEL (NOEL):** NOAEL = 1000 mg/kg/day

**Actual dose received by dose level by sex if known:** Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day.

**Remarks:** There was little evidence of toxicity noted in animals treated at levels up to 1000 mg/kg/day. A slight increase in male body weight was noted at 1000 mg/kg but the increase did not achieve statistical significance. Statistically significant, but equivocal changes in urinary volume (higher than controls) and kidney weight (lower than controls) were considered unlikely to be treatment related in the absence of any macro- or microscopic changes. There were no treatment related findings associated with treatment at 25 or 150 mg/kg/day.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint.

**References:** Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

## B. Test Substance

**Identity (purity):** CAS No. 1120-36-1, 1-Tetradecene

Remarks: Blend of three suppliers' 1-tetradecene, 99% purity

### Method

Method/guideline: OECD 422  
Test type: Combined repeated dose toxicity study with reproduction/developmental toxicity screening test

GLP: Yes  
Year: 1995  
Species: Rat  
Strain: Sprague-Dawley  
Route of Administration: Oral gavage

Duration of test: Up to 51 days; see Remarks  
Doses: 0, 100, 500, or 1000 mg/kg b.w./day  
Sex: Males and females  
Exposure period: Up to 51 days, see Remarks  
Frequency of treatment: Once daily

Control group and treatment: Concurrent vehicle control (corn oil)

Post exposure observation period: None

Statistical methods: Continuous data, including body weights, body weight gain, food consumption, clinical pathology data, organ weights, forelimb and hindlimb grip strength, landing footsplay and motor activity were analyzed by One-Way Analysis of Variance. If significance was detected, group by group comparisons were performed using Dunnett's test. All analyses utilized two-tailed tests for a minimum significance of 5% comparing the control group to the treated groups.

**Test Conditions:** This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Sprague Dawley rats. At study initiation, the males were 6 wks of age and weighed 159-220 g; the females were 8 wks of age and weighed 184-242 g (satellite) and 158-215 g (breeding). The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred.

Doses were selected based on the results of a 14-day rangefinding study. Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day, administered in a volume of 5 ml/kg. Animals were observed daily for signs of toxicity. Male and satellite female body weights were measured weekly throughout the study. Breeding female body weights were also measured weekly, prior to mating. When positive evidence of mating was detected for these females, body weights were measured on gestation days 0, 7, 14, and 20 and lactation days 1 and 4. Body weights for mated females with no evidence of copulation were measured weekly until euthanasia. Food consumption was measured on the same days as the body weights, except during the cohabitation period. Breeding females were allowed to deliver and raise offspring until lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Selected F0 males and all satellite females were evaluated for motor activity, clinical pathology, and functional observational battery before euthanasia. The liver, kidneys, testes/ovaries, adrenal glands, thymus, spleen, brain and heart of each animal were weighed. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues (accessory genital organs, adrenals, aorta, brain, cecum, colon, duodenum, esophagus, exorbital lachrymal glands, eyes with optic nerve, femur, heart, ileum, jejunum, kidneys, liver, lungs, mammary gland, mesenteric lymph node, pancreas, peripheral nerve, pituitary, rectum, skeletal muscle, skin, spinal cord, spleen, sternum with bone marrow, stomach, submaxillary salivary gland, testes or ovaries, thymus, thyroid, parathyroid, tongue, trachea, and urinary bladder) from five randomly selected males and satellite females from the control and high dose groups; the lungs, liver, kidneys, and reproductive organs [female only] from an additional 3 males and 3 satellite females from the control and high dose groups and from 8 males and 8 satellite females from the 100 mg/kg/day and 500 mg/kg/day groups).

## Results

NOAEL (NOEL): NOEL = 100 mg/kg/day (systemic) for females (liver effects); none for males due to kidney effects  
NOEL = 1000 mg/kg/day (neurotoxicity)  
LOAEL = 500 mg/kg/day for females and 100 mg/kg/day for males

Actual dose received  
by dose level by  
sex if known:

As administered. Analysis of dosing mixtures confirmed that mixtures were accurately prepared.

Remarks:

Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals.

Dose-related hydrocarbon nephropathy was noted in kidneys of male rats in all groups. The changes consisted of an increased incidence of large,

angular or rhomboid eosinophilic hyaline droplets in the proximal convoluted tubules of the kidneys.

	0 mg/kg/day	100 mg/kg/day	500 mg/kg/day	1000 mg/kg/day
Hyaline droplets - minimal	0	1	2	1
Hyaline droplets - mild	0	1	1	0
Hyaline droplets - moderate	1	2	0	3

Male and female rat livers showed minimal-to-mild hepatocyte cytoplasmic vacuolation in the 500 (3/8 males and 5/8 females) and 1000 mg/kg/day (4/8 males and 4/8 females) groups.

This was associated with increases in liver weights (see values below for doses of 0, 100, 500, and 1000 mg/kg/day; \* = statistically significant [p<0.05]; \*\* = statistically significant [p<0.01]):

- Absolute liver weight, male (g, mean±SD): 15.70±2.16, 16.98±2.04, 18.44±2.02\*, 18.29±0.76\*
- Absolute liver weight, female (g, mean±SD): 9.93±0.91, 10.76±1.21, 11.83±1.31\*, 12.90±1.49\*\*
- Organ weight/brain weight ratio (g/100g; mean±SD), male: 697.6±70.0, 746.0±71.4, 800.9±82.5\*, 788.9±57.0\*
- Organ weight/brain weight ratio (g/100g; mean±SD), female: 474.2±51.1, 504.5±55.4, 542.5±60.9, 596.2±73.9\*\*

There were no test article-related differences in the functional observational battery and motor activity tests that would indicate neurotoxicity. The NOEL for neurotoxicity was 1000 mg/kg/day in males and females. For systemic effects, the NOEL was 100 mg/kg/day in the satellite females. Since hydrocarbon nephropathy was seen in all male dose groups, there was not a NOEL for male rats for systemic toxicity. However, male rat hydrocarbon nephropathy is unique to the male rat, and does not suggest an adverse effect for human risk assessment.

(See sections 5.9 A and B for Reproductive and Developmental results)

- Reliability:** (1) Reliable without restrictions.
- Flag:** Key study for SIDS endpoint.
- References:** Daniel, E.M. (1995) Combined Repeated Dose Toxicity Study/Reproduction/Developmental Toxicity Screening Test in Rats with 1-Tetradecene. Conducted by Springborn Laboratories, Inc., Spencerville, Ohio, Study No. 3325.2 for the Chemical Manufacturers Association, Alpha Olefins Panel.
- Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

### C. Test Substance

Identity (purity): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

### Method

Method/guideline:

Test type: Subacute toxicity

GLP: Yes

Year: 1983

Species: Rat

Strain: Fischer 344

Route of

Administration: Dermal

Duration of test: 2 weeks

Doses: 0, 1.0, and 2.0 g/kg/day

Sex: Males and females

Exposure period: 2 weeks

Frequency of treatment: Once daily for 9 doses over 2-wk period

Control group and treatment:

Concurrent vehicle control (5 M, 5 F, corn oil)

Post exposure

observation period: None

Statistical methods:

Organ weights: Bartlett's test and one-way analysis of variance; if the Bartlett's test indicated the data were homogeneous, Dunnett's test was also performed; if the Bartlett's test indicated the data were non-homogeneous, a modified t-test was performed. Histopath: Kolmogorov-Smirnov Two-Tail Test (0.05 level of significance)

### Test Conditions:

Animals were approximately 7 weeks of age and weighing 90-120 g at study initiation. Prior to treatment, the backs of all animals were clipped free of hair. To prevent ingestion of the test substance, each animal was fitted with an Elizabethan collar. The collar remained on the animals until removal of residual test/control substance. Dermal doses of 2.0 g/kg (undiluted) or 1.0 g/kg (diluted 1:1 with corn oil prepared weekly) of GULFTENE 12-16 were administered to groups of 5 males and 5 female Fischer 344 rats, in 9 daily doses over a 2-wk period. An equivalent volume of the

vehicle was administered to the control group. The treated area was approximately 10% of the body surface. Approximately 6 hrs following each application, residual test substance was wiped from the application site. Parameters evaluated for treatment-related effects included survival; body weight (weekly); food consumption (weekly); appearance and behavior (at least once daily on dosing days); dermal reaction (according to the method of Draize on each dosing day prior to dosing and after removal of residual material); hematology (blood samples collected via orbital sinus) and clinical chemistry (collected prior to treatment and necropsy); organ weights, organ weight ratios relative to body and brain weights (liver, brain, spleen, heart, kidney, testes); gross pathology, and microscopic pathology (control and high-dose animals only: lungs, skin, liver, brain, spleen, heart, kidney, testes, ovaries). All animals were sacrificed approximately 24 hrs after the ninth treatment by inhalation of methoxyflurane.

## Results

NOAEL (NOEL): 1g/kg/day (systemic) [By summary author – study authors did not declare a NOAEL]

Remarks: All animals survived to the end of the study and no moribund animals were observed during the study.

Repeated application of undiluted GULFTENE 12-16 at 2.0 g/kg produced severe erythema (beet redness) to slight eschar formation (injuries in depth) and slight edema (edges of area well defined by definite raising) in all animals. Dermal reactions increased in severity with the number of applications. In all animals, slight to moderate desquamation was detected after the second treatment and persisted until the end of treatment. Slight to moderate hair loss was detected in 8/10 animals after the eighth treatment. Fissuring was also noted in 4 female animals after 6 treatments.

When GULFTENE 12-16 was administered at a 1.0 g/kg level, 2 males exhibited very slight erythema (barely perceptible) after 6 treatments and a third male after seven treatments. In one of the 3, the intensity of the erythema increased to slight and a pinpoint spot of eschar was observed after the seventh treatment. All reactions persisted throughout the study period. No edema or other reactions were noted.

In comparison to controls, depressed body weight gains were observed in the 2.0 g/kg group but not in the 1.0 g/kg group. In the 2.0 g/kg group, means for males and females increased by 25.6 g and 22.8 g, respectively, while means for control males and females increased by 52.3 g and 28.8 g, respectively, over the study period.

In the 2.0 g/kg group, the decreases in bodyweight were associated with decreases in the absolute weights of most organ systems (mean, treated vs control):

- liver: males = 6.35 g vs 7.99 g [p = 0.01]
- brain: females = 1.56 g vs 1.60 g [p = 0.05]
- spleen: males = 0.39 g vs 0.43 g [p = 0.05]
- heart: males = 0.55 g vs 0.65 g [p = 0.01]
- kidney, left: males = 0.59 g vs 0.64 g [p = 0.05]
- kidney, right: not sig. different from control
- testes: not sig. diff. from control

In the 2.0 g/kg group, the changes in body and organ weights resulted in statistically significant differences in the relative weight ratios for several organs (mean ratio in treated vs control):

- brain: males = 1.24 vs 1.04 [p = 0.01]
- spleen: males = 0.29 vs 0.27 [p = 0.01] and females = 0.32 vs 0.29 [p = 0.01]
- kidney, left: males = 0.45 vs 0.40 [p = 0.01] and females = 0.47 vs 0.42
- kidney, right: males = 0.45 vs 0.39 [p = 0.01] and females = 0.47 vs 0.43 [p = 0.05]
- testes: not sig. diff. from control

In the 2.0 g/kg group, the changes in body and organ weights resulted in statistically significant differences in the organ/brain weight ratios (mean ratio in treated vs control):

- liver: males = 3.97 vs 4.78 [p = 0.05]
- heart: males = 0.33 vs 0.39 [p = 0.05]
- kidney, left: males = 0.36 vs 0.38 [p = 0.05]

No treatment related effects were noted for food consumption, clinical signs (other than dermal reactions), hematology, and clinical chemistry. Treatment was associated with histological changes in the skin at the point of application in all animals. There were no other microscopic changes seen that could be associated with the test substance.

Study authors concluded that, under conditions of the study, repeated dermal applications of GULFTENE 12-16 at 2.0 g/kg, but not at 1.0 g/kg, caused severe skin reactions and depressed body weight gains.

**Reliability:**

(1) Reliable without restrictions.

**Flag:**

Key study for SIDS endpoint.

**References:** Gulf Life Sciences Center (1983) Two-Week Repeated Dose Toxicity Study in Rats Using GULFTENE 12-16, Project No. 82-059. Conducted for Gulf Oil Chemicals Company (unpublished report).

## 5.6 Genetic Toxicity *in vitro*

### A. Gene Mutation

#### (1) Test Substance

**Identity (*purity*):** CAS# 629-73-2, 1-hexadecene (Alpha-olefin fraction C16, min. 90.6%; vinylidenes, max.. 7.5%; internal olefins, max. 2%; paraffins, max.1.5%)

#### Method

**Method/guideline:** Maron, Ames Assay, according to OECD Guideline 471  
**Type:** in-vitro bacterial reverse mutation – Ames Assay  
**System of testing:** bacterial  
**GLP:** No  
**Year:** 1990  
**Species/Strain:** *Salmonella typhimurium* TA97A, TA98, TA100  
**Metabolic activation:** With and without S9 fraction (20 ul/plate) of livers from rats induced with Delor 105 (a mix of chlorinated hydrocarbons)  
**Concentrations tested:** 0, 10, 20, 50, 100, and 200 µl/plate  
**Statistical Methods:** The two-fold increase modified rule was used for evaluation of results. To be declared positive, the results must have shown a two-fold increase in revertants, compared to control, and a dose response.

**Test Conditions:** Undiluted test material was added directly to Petri dishes at the following doses: 0, 10, 20, 50, 100, and 200 µl per dish. For better emulsification, 50 µl of Tween 80 was added to each agar dish. The genotype of the test strains was verified (uvr B mutation, rfa mutation, presence of plasmid pKM 101). Negative and positive control experiments were included. In negative controls, the top-agar with Tween 80 was used. Strain specific positive controls were used: nitro-o-phenylenediamine (for TA97 and TA98), sodium azide (TA 100) and 2-aminofluorene (for metabolic activation experiments with all three strains). A confirmatory assay was performed. Three plates were used per dose level. Protocol deviation: only 3 of the 4 strains recommended by OECD 471 were used.

#### Results

**Cytotoxic conc.:** No data  
**Genotoxic effects:** Negative with and without metabolic activation

**Remarks:** The test material did not produce any evidence of mutagenicity in any strain.

**Reliability:** (2) Reliable with restrictions; TA 1535 was not tested.

**Flag:** Key study for SIDS endpoint.

**References:** Research Institute of Organic Synthesis a.s (1990). Pardubice, Czech Republic, Report No. T2129 (unpublished report).

(2) **Test Substance**

**Identity (purity):** C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

**Remarks** Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

**Method**

**Method/guideline:** Equivalent to OECD 476 except that a confirmatory assay was not conducted

**Type:** Mammalian cell HGPRT gene mutation assay

**System of testing:** non-bacterial

**GLP:** Yes

**Year:** 1982

**Species/Strain:** Chinese Hamster Ovary Cell (CHO-K1) received from Dr. J.P. O'Neill, Oak Ridge National Laboratories, Oak Ridge, Tennessee.

**Metabolic activation:** With and without S9 fraction of livers from rats pretreated with Aroclor 1254; protein concentration = 10 mg/ml; 0.3 ml S9/flask

**Concentrations tested:** 128, 512, 1024, and 2048 ug/mL; Doses were based on a pre-test for toxicity

**Statistical Methods:** The mean and SD of the colony counts from cultures derived from each flask were computed by standard methods. Relative Survival: mean colony count in treated cultures ÷ by mean count in control cultures. Cloning Efficiency: mean colony count in each group ÷ by number of cells seeded per plate. Frequency of Mutant Colonies: ratio of total colony counts in the mutagenicity plates over total colony counts in the viability plates; group mean calculated. The frequency of mutant colonies per million clonable cells in the treated and vehicle control cultures were compared using Student's t test. A test was considered positive if there was a significant increase in mutant colonies at any dose level and a dose-related response.

**Test Conditions:** The test substance was emulsified with 10% F68 Pluronic® Polyol in water and subsequently diluted with medium to a

dosing preparation of 6% F68. Water was the vehicle for the direct acting positive control (ethylmethanesulfonate, 100 µg/ml in culture flask). DMSO was the vehicle for positive control cultures requiring metabolic activation (benzo(a)pyrene, 4 µg/ml in culture flask).

Cells were maintained in 5 ml Ham's F12 Medium (no hypoxanthine) with 5% dialyzed heat-inactivated newborn calf serum. During treatment the serum was omitted, HEPES buffer and antibiotic were included and the volume limited to 3 ml/flask. Where indicated, activating enzymes were included. After treatment, cultures were maintained in Ham's F12 (no hypoxanthine) with 5% dialyzed heat-inactivated newborn calf serum and antibiotics. For selection of mutant cells,  $10^{-5}$  M 6-thioguanine was included. Incubation was in a CO<sub>2</sub> enriched (5%) humidified (95%) atmosphere at 37.5°C except that during exposure the sealed cultures were placed in a shaker incubator at 37°C.

**RANGEFINDING:** Approx.  $5 \times 10^5$  cells seeded to each of 2 flasks/treatment (1 w/S9; 1 w/o S9); exposed to test substance at 4 – 2,048 µg/ml for 5 hrs on Day 2; on Day 3 trypsinized and counted with a Coulter Model ZB cell counter and subcultured (200 cells transferred to each of 3 60 mm culture dishes); incubated to Day 10/11; fixed in methanol and stained with Giemsa; colonies counted visually or with Artek Model 981 counter.

**MUTAGENICITY:** Each dose group was composed of 6 flasks, 3 w/S9, except that the vehicle group contained 12 flasks, 6 w/S9. The concentrations of test substance were 4, 16, 128, 512, 1024, and 2048 µg/ml. Control cultures received F68, medium, S9 mix or F68 with positive control. Sufficient cells were seeded to give approx. 1 million cells on Day 2 and exposed to test substance for 5 hrs on Day 2; on Day 3 all cultures were checked for evidence of cytotoxicity, and those showing excessive toxicity terminated. **VIABILITY:** 4 dose levels were subcultured (200 cells were transferred to each of 4 60 mm viability plates) and incubated to Day 10/11, fixed in methanol and stained with Giemsa, and colonies counted visually or with Artek Model 981 counter. **MUTAGENICITY:**  $10^5$ - $10^6$  cells seeded to 100 mm dish on Day 3 for expression; subcultured 3 times, the last on Day 10/11; 200 cells seeded to each of 4 viability plates as above, and  $2 \times 10^5$  cells seeded to each of 5 mutagenicity plates in selective medium; cultures incubated undisturbed until Day 16/18, when they were fixed and stained.

## Results

Cytotoxic conc.:  $\geq 1024$  µg/ml  
Genotoxic effects: Negative with and without metabolic activation

**Remarks:** RANGEFINDING: Some toxicity was evident at 2048 µg/mL without activation [cell count after treatment ( $\times 10^5/\text{ml}$ ) = 6.6, 6.6, 6.1, 6.4, 6.2, 5.8, 2.8 for concentrations of GULFTENE 12-16 of 0 (vehicle), 64, 128, 256, 512, 1024, and 2048 µg/ml, respectively]; and with activation [cell count after treatment ( $\times 10^5/\text{ml}$ ) = 4.1, 4.0, 2.9, 3.4, 3.4, 3.5, 2.9, 2.0 for concentrations of GULFTENE 12-16 of 0 (vehicle), 32, 64, 128, 256, 512, 1024, and 2048 µg/ml, respectively]. Toxicity was within acceptable limits.

DEFINITIVE TEST: A toxic effect was noted in that there were insufficient cells after treatment to subculture at  $1 \times 10^6$  per dish at the 1024 and 2048 levels without activation and that cultures with activation also showed immediate toxicity at those levels [cell counts after treatment ( $\times 10^5/\text{ml}$ ) = 5.1, 5.1, 4.4, 2.8, and 2.1 at concentrations of 0 (vehicle), 128, 512, 1024, and 2048 µg/ml, respectively]. Colony counts after subculture showed that cells which were used to determine the mutagenic effect were able to grow and had recovered from the initial toxic effect. Cloning Efficiency after treatment = 64% and 56% at 2048 µg/ml (w/o and w/S9, respectively). Relative Survival after treatment = 83% and 68% at 2048 µg/ml (w/o and w/S9, respectively). Cloning Efficiency after expression = 82% and 86% at 2048 µg/ml (w/o and w/S9, respectively). Relative Survival after expression = 97% and 100% at 2048 µg/ml (w/o and w/S9, respectively). The frequency of mutant colonies was increased to expected values in the two positive control groups indicating the assay was functional. There were no increases over control in frequency of mutant colonies when cultures were treated with test article.

**Reliability:** (2) Reliable with restrictions: Confirmatory assay was not conducted

**References:** Gulf Life Sciences Center, Pittsburgh, Pennsylvania (1983) CHO/HGPRT Test: GULFTENE 12-16, Project 82-102. Conducted for Gulf Oil Chemicals Company (unpublished study).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

## B. Chromosomal Aberration

### Test Substance

Identity (*purity*): CAS No. 2437-56-1, 1-Tridecene and CAS No. 1120-36-1, 1-Tetradecene (SHOP Olefin C13/14; not further characterized)

## Method

Method/guideline: no data  
Type: in-vitro mammalian cell chromosome aberration test  
System of testing: non-bacterial  
GLP: no data  
Year: 1982  
Cell line: Rat liver RL1 cells

Metabolic activation: With and without S9 fraction from rat liver

Concentrations tested: no data

Statistical Methods: no data

**Test Conditions:** no data

## Results

Cytotoxic conc.: There was no cytotoxicity  
Genotoxic effects: Negative with and without metabolic activation

**Reliability:** (4) Not assignable; limited information available

**References:** Brooks, T.M. (1982) Toxicity of detergents/higher olefins: In vitro genotoxicity studies on SHOP products (olefin C11/12 and C13/14, olefin HE bleed and olefin intermediate recycle). Shell Research Limited, Sittingbourne (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

## C. Other Genetic Effects

### (1) Test Substance

Identity (*purity*): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

### Method

Method/guideline: OECD 482 except that independent repeat was not conducted  
Type: In-vitro unscheduled DNA synthesis  
System of testing: Non-bacterial  
GLP: Yes  
Year: 1984

Cell line: Primary rat hepatocytes  
Metabolic activation: None  
Concentrations tested: Rangefinding experiment: 8, 16, 32, 64, 128, 256, 512, 1024, 2048 and 5000 ug/ml  
UDS experiment: 100, 1000, 2000 and 4000 ug/ml  
Statistical Methods: The test substance was considered positive for unscheduled DNA synthesis (UDS) when the mean net nuclear grain count at any treatment level exceeded that of the concurrent negative control by at least 6 grains per nucleus, and the value for the negative control did not exceed 5. A dose response was not needed.

**Test Conditions:** Primary cultures of hepatocytes from livers of freshly perfused F344 rats were exposed to the test substance in the presence of <sup>3</sup>H-thymidine. Cytotoxicity was evaluated in a separate assay and used as a basis for dosage selection. The occurrence of UDS was visualized autoradiographically and quantified with the aid of microscopy.

A 10% solution of Pluronic® F68 Polyol in water was used to emulsify the test substance. This was diluted with medium so that the concentration of F68 in the dosing preparations was 3.5% . Dosing preparations were added to the cultures in aliquots of 30 or 50 ul. This produced a culture concentration of 0.035% F68. The positive control was 2-acetylaminofluorene (2-AAF) prepared using DMSO and Pluronic F68 Polyol and administered at 0.2 ug/ml 2-AAF in the final culture.

The cells were grown in 3 ml (UDS) or 5 ml (rangefinding) Williams Medium E supplemented with 10% fetal bovine serum and insulin. Antibiotics were included. During the exposure period, 0.1M HEPES buffer, 2% by volume, and 0.1N HCL, 1% by volume, were present in the medium. The cells were cultured in plastic vessels. Incubation was in a carbon dioxide-enriched (5%), humidified atmosphere at 37°C. During the exposure period, cultures were sealed.

**RANGEFINDING EXPERIMENT:** In the rangefinding experiment, hepatocytes were harvested from one male rat aged 11 weeks and weighing 250 g. Two cultures each were prepared for the negative control, vehicle control and 10 levels of test substance. Approximately  $1 \times 10^5$  cells/ml were seeded into each treatment culture and exposed to the test substance for 18 hours. The cells were then stained with trypan blue, fixed with formalin, and counted for viability determination. The culture vessel was taken as the experimental unit. The average number of viable cells per treatment group was determined. The relative viability was then calculated as the average number of viable cells in substance-treated cultures divided by that in the vehicle control cultures. For the evaluation of toxicity, at least 50%

viability was desired. The final choice of treatment levels was based on the expectation that at least one level showed toxicity.

**UDS EXPERIMENT:** In the UDS experiment, hepatocytes were harvested from 1 male rat aged 13 weeks and weighing 270 g. Three cultures each were prepared for the negative control, vehicle control, positive control, and 4 levels of test substance. Approximately  $1 \times 10^5$  cells/ml were seeded into each treatment culture and exposed to  $^3\text{H}$ -thymidine and test substance for 18 hours. Cells growing on coverslips were rinsed, exposed to hypotonic solution, fixed, air dried and glued to microscope slides on Day 2. On Day 3, the slides were dipped in autoradiographic emulsion and stored in the dark at 2-8°C. Autoradiographs were developed, stained and coverslipped on Day 13. The number of grains overlying each of 50 randomly selected nuclei per slide was counted microscopically. The highest of 3 cytoplasmic grain counts per cell was subtracted to obtain the net nuclear grain count. The individual slide was taken as the experimental unit. The average net nuclear grain count per slide (sum of net nuclear grain counts divided by 50) was calculated and the mean net nuclear grain count (average net nuclear grain count per slide divided by 3) was determined for each treatment level.

**Results**

Cytotoxic conc.: 256 µg/ml

Genotoxic effects: Negative

Remarks: In the rangefinding experiment, GULFTENE 12-16 was toxic to primary hepatocytes beginning at 256 µg/ml where 74% relative viability was observed following an 18-hr exposure period. Cytotoxicity increased only slightly with increasing dose to 2048 µg/ml and then increased sharply at the highest dose tested, 5000 µg/ml, where a relative viability of 45.1% was observed. In the UDS experiment, both positive and negative controls gave the expected responses. No treatment level elicited a positive response for UDS.

Reliability: (2) Reliable with restrictions: Confirmatory assay not conducted

References: Gulf Life Sciences (1984) Hepatocyte Primary Culture/DNA Repair Test of GULFTENE12-16, project #2069 (unpublished report).

Other: This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

(2) **Test Substance**

**Identity (purity):** C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

**Remarks** Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

**Method**

**Method/guideline:** Equivalent to US EPA TSCA 40 CFR 795.285 and ECC B21, except that a confirmatory assay was not conducted

**Type:** BALB/3T3 Transformation Test

**System of testing:** Non-bacterial

**GLP:** No

**Year:** 1983

**Cell line:** Mouse embryo cells, BALB/3T3-A31-1-1

**Metabolic activation:** None

**Concentrations tested:** Rangefinding experiment: 8, 16, 32, 64, 128, 256, 512, 1024, 2048 and 5000 µg/ml  
Transformation experiment: 10, 20, 30 and 1500 µg/ml

**Statistical Methods:** A test was considered positive if there were: 1) a two-fold increase in Type-III foci at the highest dose over that seen in vehicle control cultures, with or without a dose-related response or 2) a two-fold increase at two or more consecutive dose levels. Where vehicle control cultures have no Type-III foci, at least 2 foci would be needed for a dose level to be considered positive.

**Test Conditions:** Cytotoxicity was evaluated in a separate assay and used as a basis for dosage selection.

A 10% solution of Pluronic® F68 Polyol in water was used to emulsify the test substance. This was diluted with medium so that the concentration of F68 in the dosing preparations was 3.5%. Dosing preparations were added to the cultures in aliquots of 50 µl. This produced a culture concentration of 0.035% F68. The positive control was 3-methylcholanthrene (3-MC) prepared using DMSO and Pluronic® F68 Polyol and administered at 1 µg/ml 3-MC in the final culture.

The cells were received from Dr. Takeo Kakunaga, National Cancer Institute, at Passage 14 after origination of the subclone. The cells were subcultured once, tested for presence of adventitious infectious agents and for capability to respond to known transforming agents, and frozen. Cultures used in testing were less than 4 additional passages from frozen stock. The cells were grown in 5 ml Eagle's Minimum Essential Medium supplemented with 10% heat-inactivated fetal calf serum. Antibiotics were included. Incubation was in a carbon dioxide-enriched (5%), humidified atmosphere at 37°C.

**RANGEFINDING EXPERIMENT:** Each treatment group (medium, vehicle, and 10 levels of test substance) consisted of two cultures. Approximately  $1 \times 10^4$  cells were seeded into each treatment flask on Day 1. The cultures were exposed to the test substance for 2 days, beginning on Day 2, then trypsinized and counted on Day 4 with a Coulter Model ZB cell counter. The culture vessel was taken as the experimental unit. The average number of surviving cells per treatment group was determined. The relative survival was then calculated as the average number of surviving cells in substance-treated cultures divided by that in the vehicle control cultures. For the evaluation of toxicity, at least 20% survival was desired. The final choice of treatment levels was based on the expectation that at least one level showed toxicity.

**TRANSFORMATION EXPERIMENT:** Each group (medium control, vehicle control, positive control, and 4 levels of test substance) consisted of 15 flask cultures for transformation and 2 flask cultures for cloning. Transformation flasks were seeded with approximately  $1 \times 10^4$  cells and cloning flasks with approximately 100 cells on Day 1. The cells were exposed to test substance for 2 days beginning on Day 2. The medium was changed on all cultures on Day 4. Cloning cultures were fixed and stained for colony counting on Day 8. Colonies (at least 50 cells) were counted visually and, where required, examined microscopically. The medium was changed weekly on all transformation flask cultures. Fixation and staining of flask cultures for focus counting and evaluation were on day 29. Foci were counted visually and examined microscopically to determine type.

The cloning efficiency was determined by dividing the average number of colonies (at least 50 cells) per flask by the number of cells seeded and converting to a percent. The relative cloning efficiency was determined by dividing the cloning efficiency for each treatment group by the cloning efficiency for the vehicle control, and converting to a percent. The transformation frequency for each group was the total number of Type III foci divided by the total number of flasks per group.

**Results:**

Cytotoxic conc.: Concentrations of  $>20 \mu\text{g/ml}$  were cytotoxic  
Genotoxic effects: Negative

Remarks: In the rangefinding experiment, GULFTENE 12-16 was toxic to BALB/3T3 cells at  $32 \mu\text{g/ml}$  when 16% viability was observed following a 2-day exposure period. Viability remained at this level up to a dose of  $2048 \mu\text{g/ml}$ . At  $5000 \mu\text{g/ml}$ , the relative viability was reduced to 1.3%.

In the transformation experiment, cloning efficiency was used as a measure of toxicity. Toxicity became evident at 20 µg/ml (27% relative cloning efficiency) and remained near this level through the highest dose tested, 1500 µg/ml.. The positive control gave the expected response. The negative controls were within acceptable limits for the test. No treatment level exceeded the medium controls for Type III foci. Under the conditions of the test, GULFTENE 12-16 was negative for cell transformation.

**Reliability:** (2) Reliable with restrictions: Confirmatory assay not conducted

**References:** Goode, J.W. and Brecher, S. (1983) GULFTENE 12-16: BALB/3T3 transformation test, Project 2070. Sponsored by Gulf Life Sciences Institute, Pittsburg, PA (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

(3) **Test Substance**

**Identity (purity):** CAS No. 2437-56-1, 1-Tridecene and CAS No. 1120-36-1, 1-Tetradecene (SHOP Olefin C13/14; not further characterized)

**Method**

**Method/guideline:** no data  
**Type:** Mitotic Gene Conversion  
**System of testing:** non-bacterial  
**GLP:** yes  
**Year:** 1982  
**Species/Strain:** Saccharomyces cerevisiae JD1  
**Metabolic activation:** no data  
**Concentrations tested:** no data  
**Statistical Methods:** no data

**Test Conditions:** no data

**Results**

**Cytotoxic conc.:** no data  
**Genotoxic effects:** Negative

**Remarks:** There was no increase in mitotic gene conversion in *Saccharomyces cerevisiae*

**Reliability:** (4) Not assignable: limited information available.

**References:** Brooks, T.M. (1982) Toxicity of detergents/higher olefins: In vitro genotoxicity studies on SHOP products (olefin C11/12 and C13/14, olefin HE bleed and olefin intermediate recycle). Shell Research Limited, Sittingbourne (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11.

## 5.7 Genetic Toxicity *in vivo*

### A. Test Substance

Identity (purity): CAS# 629-73-2, 1-hexadecene (Alpha-olefin fraction C16, min. 90.6%; Vinylidenes, max.. 7.5%; internal olefins, max. 2%; paraffins, max.1.5%)

### Method

Method/guideline: OECD Guideline 474  
Type: Micronucleus Test  
GLP: No  
Year: 1990  
Species: Mouse  
Strain: Random bred strain ICR-SPF (Velaz Prague)  
Sex: Male and female  
Route of Administration: Oral gavage  
Concentration levels: 7.85 g/kg - undiluted  
Exposure period: Single dose, sampled at 24, 48 and 72 hrs after test substance administration, and 48 hrs after administration of negative and positive controls  
Statistical methods: Statistical evaluation was done according to tables of mutation frequencies (Kastenbaum and Bowman, 1970). Sexes were analyzed separately.

**Test Conditions:** The mice were housed in conventional animal housing with natural light-dark cycle in plastic cages. The mice were fed standard pelleted diet (VELAZ, Prague) and tap water (quality for human consumption).

The maximum tolerated dose was determined by a rangefinding experiment (0.1 ml test substance per 10 g of animal weight with sacrifice at 72 hrs). No adverse effects were observed, so the dose for testing was determined by physical properties of 1-hexadecene.

For the mutagenicity test, animals (5 male and 5 female per group) were 8-12 wks of age at study initiation. The test material was administered by oral gavage in a single dose at a concentration of 7.85 g/kg (maximum tolerated dose) to 15 mice/sex. The positive control, benzene (2 g/kg and 4 g/kg), was administered by oral gavage as a single dose to 5 mice/sex. The concurrent negative control group (5 mice/sex) received olive oil (0.1 ml/10 g body weight). Test material treated animals (5 animals/sex/group) were sacrificed at approximately 24, 48 and 72 hours after dose administration. Animals dosed with olive oil and benzene

were sacrificed at 48 hours only. Bone marrow was obtained from both femurs. Bone marrow smears were prepared and stained with Giemsa. 1000 polychromatic erythrocytes (PCE) per animal were scored for micronuclei. The ratio of PCE to normochromatic erythrocytes (NCE) was determined by counting 200 erythrocytes per animal.

## Results

### Effect on

PCE/NCE ratio: A decrease in PCE/NCE ratio was observed

Genotoxic effects: Negative

NOEL: 7.85 g/kg

Remarks: There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, indicating that the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control is clastogenic. In addition, the test material induced decreases in the mean percent of polychromatic erythrocytes, which is a measure of bone marrow toxicity. A highly positive response was obtained with the positive control substance.

Sex	Dose (g/kg)	Interval (hrs)	No. PCE	MNPCE/1000 PCE		PCE/(PCE+NCE)
				mean	SD(%)	
Male	7.85	24	5000	1.4	2.2	45.0
		48	5000	1.8	1.6	45.0
		72	5000	1.0	1.2	48.1
	olive oil	48	5000	1.2	0.8	48.6
Female	7.85	24	5000	1.2	1.1	48.3
		48	5000	0.8	1.1	43.3
		72	5000	0.8	0.8	42.9
	olive oil	48	5000	0.6	0.9	49.3

Reliability: (2) Reliable with restrictions: no GLP

Flag: Key study for SIDS endpoint

References: Research Institute of Organic Synthesis a.s (1990). Pardubice, Czech Republic Project No. T2129 (unpublished report).

## B. Test Substance

Identity (purity): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

**Remarks** Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

### **Method**

**Method/guideline:** Equivalent to OECD 474  
**Type:** Micronucleus Assay  
**GLP:** Yes  
**Year:** 1982  
**Species:** Mouse  
**Strain:** Crl: Cd-1 (ICR) BR Swiss  
**Sex:** Male and female  
**Route of Administration:** Dermal  
**Concentration levels:** 1000, 2500 and 5000 mg/kg. Concentrations were based on the results of a range-finding study.  
**Exposure period:** 2 days  
**Statistical methods:** The group mean bodyweight was calculated for each day. The treatment and group means were compared using Student's t test. The group means and standard deviations for polychromatic erythrocytes (PCE) with micronuclei, and the group mean ratio of PCE to normochromatic erythrocytes (NCE) were calculated. Values from treated groups were compared with values from the vehicle control group using Student's t test. The test would be considered positive if there were a significant increase in micronucleated PCE at any dose level, and if a dose-related response were evident.

**Test Conditions:** Animals were 11 wks of age at start of treatment and weighed 28-38 g (males) and 22-30 g (females). Test article was administered undiluted. Negative control in the test was corn oil; cyclophosphamide was positive control. Test article was applied at a maximum volume of 0.2 ml on the shaved backs of the mice of Days 1 and 2. Cyclophosphamide was given by intraperitoneal injection at a dose of 75 mg/kg. Cyclophosphamide-treated animals were sacrificed on day 3; other groups were sacrificed on days 3 and 4 and bone marrow smears were prepared. Smears were stained with May-Grunwald and Giemsa stains and examined microscopically. Approximately 1000 PCEs and all NCEs in the scan path were observed for each animal. Animals were weighed on Days 1, 3 and 4 and observed daily.

### **Results**

**Effect on PCE/NCE ratio:** Results not reported  
**Genotoxic effects:** Negative.

**NOEL:** 5.0 g/kg

**Remarks:** All animals (5 per sex per group) survived to sacrifice. There were no remarkable clinical findings, or effects on body weight changes. Slides from animals given corn oil and cyclophosphamide gave expected results. Slides from animals given GULFTENE C12-16 gave no significant increase (T-test,  $p < 0.05$ ) in micronucleated bone marrow erythrocytes or dose related response.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Gulf Life Sciences Center, Pittsburgh, Pennsylvania (1983)  
Micronucleus Test in Mouse Bone Marrow with GULFTENE 12-16 Administered by Dermal Application for 2 Days. Gulf Oil Chemicals Company, Sponsor (unpublished report).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

## 5.8 Carcinogenicity

**Remarks:** No long-term carcinogenicity tests have been conducted on long-chain alpha olefins. However, there are no structural indicators to suggest carcinogenicity. For analogy, long-term carcinogenicity studies have been conducted for alpha olefin sulfonates (AOS) derived from alpha olefins of similar alkyl length. For example, Hunter and Benson (1976) fed rats mixed C<sub>14-16</sub> AOS at dietary levels of 1000, 2500, and 5000 ppm for two years. Blood chemistries, urinalyses, and histopathological findings were comparable to control values. There was no increase in tumors from the feeding of the test article. Three carcinogenicity studies of AOS reported by Oba and Takei (1992) indicated that these AOS were not carcinogenic by oral or dermal routes.

**References:** Hunter B., and H.G. Benson (1976) Long-term toxicity of the surfactant alpha-olefin sulphonate in the rat. *Toxicology* 5:359-370.

Oba, K. and R. Takei (1992) Carcinogenic, mutagenic/genetic toxicity and teratogenic properties. Chapter 7, pp. 331-409, in *Anionic Surfactants: Biochemistry, Toxicology, and Dermatology*, 2nd edition, Eds. C. Gloxhuber and K. Kuenstler, Surfactant Science Series, Vol. 43, Marcel-Dekker, Inc., New York.

**Other:** These remarks were included in the dossier for 1-tetradecene at SIAM 11.

## 5.9 Reproductive Toxicity (including Fertility and Developmental Toxicity).

### A. Fertility

**(1) Test Substance**

Identity (purity): CAS No. 1120-36-1, 1-Tetradecene (99%)

Remarks: Blend of three suppliers' 1-tetradecene

**Method**

Method/guideline: OECD 422 (see Section 5.5B for general toxicity endpoints and Section 5.9B for developmental toxicity endpoints)

Type: Combined Repeated Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test

GLP: Yes

Year: 1995

Species: Rat

Strain: Sprague-Dawley

Route of administration: Oral gavage

Concentration levels: 0, 100, 500, 1000 mg/kg/day

Sex: Male and female

Control group and treatment: Corn oil by oral gavage

Frequency of treatment: Daily

Exposure period: Up to 51 days; see Remarks

Duration of test: Through lactation day 4 for pups

Premating exposure period for males: 4 weeks

Premating exposure period for females: 2 weeks

Statistical methods: Continuous data, including body weights, body weight gain, food consumption, clinical pathology data, organ weights, gestation length, mean live litter size, implantation scar counts, were analyzed by One-Way Analysis of Variance. If significance was detected, group by group comparisons were performed using Dunnett's test. Count data were analyzed utilizing Chi-Square test for copulation and fertility indices, pup sex ratios, the number of live and dead pups per group on lactation day ) and pup survival after lactation day 0. All analyses utilized two-tailed tests for a minimum significance of 5% comparing the control group to the treated groups.

**Test Conditions:** This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Sprague Dawley rats. At study initiation, the males were 6 wks of age and weighed 159-220 g; the females were 8 wks of age and weighed 184-242 g (satellite) and 158-215 g (breeding). The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating,

during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred

Doses were selected based on the results of a 14-day rangefinding study. Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day, administered in a volume of 5 ml/kg. Animals were observed daily for signs of toxicity. Male and satellite female body weights were measured weekly throughout the study. Breeding female body weights were also measured weekly, prior to mating. When positive evidence of mating was detected for these females, body weights were measured on gestation days 0, 7, 14, and 20 and lactation days 1 and 4. Body weights for mated females with no evidence of copulation were measured weekly until euthanasia. Food consumption was measured on the same days as the body weights, except during the cohabitation period. Breeding females were allowed to deliver and raise offspring until lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Selected F0 males and all satellite females were evaluated for motor activity, clinical pathology, and functional observational battery before euthanasia. The liver, kidneys, testes/ovaries, adrenal glands, thymus, spleen, brain and heart of each animal were weighed. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues (accessory genital organs, adrenals, aorta, brain, cecum, colon, duodenum, esophagus, exorbital lachrymal glands, eyes with optic nerve, femur, heart, ileum, jejunum, kidneys, liver, lungs, mammary gland, mesenteric lymph node, pancreas, peripheral nerve, pituitary, rectum, skeletal muscle, skin, spinal cord, spleen, sternum with bone marrow, stomach, submaxillary salivary gland, testes or ovaries, thymus, thyroid, parathyroid, tongue, trachea, and urinary bladder) from five randomly selected males and satellite females from the control and high dose groups; the lungs, liver, kidneys, and reproductive organs [female only] from an additional 3 males and 3 satellite females from the control and high dose groups and from 8 males and 8 satellite females from the 100 mg/kg/day and 500 mg/kg/day groups).

## Results

NOAEL: NOAEL Parental (reproductive toxicity) = 1000 mg/kg  
NOEL for F1 offspring = 1000 mg/kg/day

Actual dose received

by dose level by sex if known: As administered. Analysis of dosing mixtures confirmed that mixtures were accurately prepared.

Maternal and Paternal general toxicity: see Section 5.5 B

Reproductive toxicity observed in parental animals: none

Reproductive toxicity observed in offspring: none

Remarks: Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals. Male and female rat livers showed hepatocyte cytoplasmic vacuolation to some degree in the 500 and 1000 mg/kg/day groups. This was associated with increases in liver weights. (See section 5.5 B for systemic and neurotoxicity results, and section 5.9 B for developmental results). There were no differences in measurements of fertility or reproductive capacity in the F0 generation, nor were there developmental effects in the F1 generation through day 4 of lactation. The NOAEL for reproductive effects was 1000 mg/kg/day in males and females.

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Daniel, E.M. (1995) Combined Repeated Dose Toxicity Study/Reproduction/Developmental Toxicity Screening Test in Rats with 1-Tetradecene. Conducted by Springborn Laboratories, Inc., Spencerville, Ohio, for Chemical Manufacturers Association, Alpha Olefins Panel, sponsor (unpublished study).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added.

(2) **Test Substance**

Identity (purity): C16/18 isomerised olefin  
 Remarks: C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%.  
 Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

**Method**

Method/guideline: OECD 407 (see Section 5.5A for general toxicity endpoints)  
 Test type: Subacute toxicity

GLP: Yes  
Year: 2000  
Species: Rat  
Strain: Sprague Dawley (crl:CD BR)  
Route of Administration: Oral gavage  
  
Duration of test: 4 weeks  
Doses: 0, 25, 150, or 1000 mg/kg./day  
Sex: Males and females  
Exposure period: 4 weeks  
Frequency of treatment: Once daily, 7 days/week  
  
Control group and treatment: Concurrent vehicle control (corn oil)  
  
Post exposure observation period: None

**Statistical methods:** Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)

**Test Conditions:** Groups of ten rats (5M:5F) were dosed orally by gavage once daily over a period of 28 days. Animals were approximately 41 days old on the first day of dosing. Animals were regularly monitored for any signs of ill health or reaction to treatment. Detailed functional observations were performed weekly, with additional functional observations performed during pretrial and week four. Animals were weighed daily to determine dose. Body weights and food consumption were recorded twice weekly. Blood and urine samples were collected during week four of the study. After four weeks of treatment animals were sacrificed and subjected to necropsy. A comprehensive list of organs were weighed and /or preserved (adrenal, brain, epididymis, eye, gastrointestinal tract including stomach, duodenum, jejunum, ileum, caecum, colon, rectum, heart, kidney, liver, lung, bone marrow, mesenteric lymph node, ovary, pituitary, prostate, sciatic nerve, spinal cord, spleen, submandibular lymph node, testis, thymus, thyroid with parathyroid, trachea, urinary bladder, uterus). Tissues from the controls and high dose animals were subjected to histological examination. Histology was also performed on the male kidneys from the lower doses.

## Results

**NOAEL (NOEL):** The NOEL for reproductive effects from limited data (effect on reproductive organs) appears to be 1000 mg/kg/day (the highest dose tested).

Actual dose received by dose level by sex if known: Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day

Remarks: Please see Repeated Dose Toxicity, Section 5.5 A for general toxicity results. There was no evidence of toxicity to reproductive organs in animals treated at levels up to 1000 mg/kg/day.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint.

**References:** Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

## B. Developmental Toxicity

### Test Substance

Identity (purity): CAS No. 1120-36-1, 1-Tetradecene (99%)

Remarks: Blend of three suppliers' 1-tetradecene

Method/guideline: OECD 422 (see Section 5.5B for general toxicity endpoints and Section 5.9A for reproductive toxicity endpoints)

Type: Combined Repeated Dose Toxicity Study with Reproduction/Developmental Toxicity Screening Test

GLP: Yes

Year: 1995

Species: Rat

Strain: Sprague-Dawley

Route of administration: Oral gavage

Concentration levels: 0, 100, 500, 1000 mg/kg/day

Sex: Male and female

Control group and treatment: Corn oil by oral gavage

Frequency of treatment: Daily

Exposure period: Up to 51 days; see Remarks

Duration of test: Through lactation day 4 for pups

Premating exposure period for males: 4 weeks

Premating exposure

period for females: 2 weeks  
Statistical methods: Continuous data, including body weights, body weight gain, food consumption, clinical pathology data, organ weights, were analyzed by One-Way Analysis of Variance. If significance was detected, group by group comparisons were performed using Dunnett's test. Count data were analyzed utilizing Chi-Square test for copulation and fertility indices, pup sex ratios, the number of live and dead pups per group on lactation day ) and pup survival after lactation day 0. All analyses utilized two-tailed tests for a minimum significance of 5% comparing the control group to the treated groups.

**Test Conditions:** This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Sprague Dawley rats. At study initiation, the males were 6 wks of age and weighed 159-220 g; the females were 8 wks of age and weighed 184-242 g (satellite) and 158-215 g (breeding). The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred

Doses were selected based on the results of a 14-day rangefinding study. Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day, administered in a volume of 5 ml/kg. Animals were observed daily for signs of toxicity. Male and satellite female body weights were measured weekly throughout the study. Breeding female body weights were also measured weekly, prior to mating. When positive evidence of mating was detected for these females, body weights were measured on gestation days 0, 7, 14, and 20 and lactation days 1 and 4. Body weights for mated females with no evidence of copulation were measured weekly until euthanasia. Food consumption was measured on the same days as the body weights, except during the cohabitation period. Breeding females were allowed to deliver and raise offspring until lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Selected F0 males and all satellite females were evaluated for motor activity, clinical pathology, and functional observational battery before euthanasia. The liver, kidneys, testes/ovaries, adrenal glands, thymus, spleen, brain and heart of each animal were weighed. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues (accessory genital organs, adrenals, aorta, brain, cecum, colon, duodenum, esophagus, exorbital lachrymal glands, eyes with optic nerve, femur, heart, ileum, jejunum, kidneys, liver, lungs, mammary gland, mesenteric lymph node, pancreas, peripheral nerve, pituitary, rectum, skeletal muscle, skin, spinal cord, spleen, sternum with bone marrow,

stomach, submaxillary salivary gland, testes or ovaries, thymus, thyroid, parathyroid, tongue, trachea, and urinary bladder) from five randomly selected males and satellite females from the control and high dose groups; the lungs, liver, kidneys, and reproductive organs [female only] from an additional 3 males and 3 satellite females from the control and high dose groups and from 8 males and 8 satellite females from the 100 mg/kg/day and 500 mg/kg/day groups).

**Results**

**NOAEL:** NOAEL for maternal toxicity = 1000 mg/kg/day  
NOAEL for teratogenicity = 1000 mg/kg/day

**Actual dose received by dose level by sex if known:** As administered. Analysis of dosing mixtures confirmed that mixtures were accurately prepared.

**Maternal and Paternal general toxicity:** See Section 5.5 B

**Remarks:** Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals. Male and female rat livers showed hepatocyte cytoplasmic vacuolation to some degree in the 500 and 1000 mg/kg/day groups. This was associated with increases in liver weights. (See section 5.5 B for systemic and neurotoxicity results, and section 5.9A for reproductive toxicity results). There were no developmental effects in the F1 generation through day 4 of lactation. The NOAEL for developmental effects was 1000 mg/kg/day (the highest dose).

**Reliability:** (1) Reliable without restrictions

**Flag:** Key study for SIDS endpoint

**References:** Daniel, E.M. (1995) Combined Repeated Dose Toxicity Study/ Reproduction/Developmental Toxicity Screening Test in Rats with 1-Tetradecene. Conducted by Springborn Laboratories, Inc., Spencerville, Ohio, for Chemical Manufacturers Association, Alpha Olefins Panel, sponsor (unpublished study).

**Other:** This study was included in the dossier for 1-tetradecene at SIAM 11. Additional information has been added. This study also appears in Section 5.9.A(2), Fertility.

**5.10 Other Relevant Information**

**A. Aspiration**

**Test Substance**

**Identity:** CAS No. 629-73-2, 1-Hexadecene

## Method

Type: General toxicity – aspiration  
Species: Rat  
Strain: Wistar  
Sex: Male  
Route of Administration: aspiration  
Dose: 0.2 mL

Results: See Remarks

Remarks: C6-C18 alkenes (even carbon numbers, alpha olefins), source and purity unspecified, were assessed for aspiration hazard in an animal study using Wistar rats. Four or five males were used per test article. Two-tenths mL of the test material was placed in the mouths of rats that had been anesthetized to the point of apnea in a covered wide mouth gallon jar containing about 1 inch of wood shavings moistened with approximately 1 ounce of anhydrous diethyl ether. As the animals began to breathe again, the nostrils were held until the test material had been aspirated or the animal regained consciousness. All alkenes tested except 1-hexene were aspirated into the lungs. 1-Hexene was difficult to dose because of its volatility. Two animals survived because the hydrocarbon “boiled” out of the mouth before it was aspirated. All animals exposed to C<sub>8</sub> to C<sub>14</sub> died within 24 hours. With C<sub>16</sub> and C<sub>18</sub>, there was only one death (C<sub>18</sub>). Lung weights were increased in alkenes-treated animals compared with controls. The affected animals showed chemical pneumonitis. The report concluded that there is a significant aspiration hazard with C<sub>6</sub> to C<sub>14</sub> alkenes.

Reference: Gerarde, H.W. (1963) Toxicological Studies on Hydrocarbons. Archives of Environmental Health, 6: 329-341.

Other: This study was included in the dossier for 1-tetradecene at SIAM 11.

## B. Neurotoxicity

### (1) Test Substance

Identity (purity): C16-18 isomerised olefin  
Remarks: C14-0.4%, C16-53.6%, C18-37.6%, C20-7.9%, C22-0.5%.  
Linear terminal 1.8%, linear internal 71.9%, Branched terminal 15.6% Trisubstituted 10.7%.

### Method

Method/guideline: OECD 407 (See Sec. 5.5.A for general toxicity endpoints)  
Test type: subacute toxicity

**GLP:** Yes  
**Year:** 2000  
**Species:** Rat  
**Strain:** Sprague Dawley (crl:CD BR)  
**Route of Administration:** Oral gavage  
  
**Duration of test:** 4 weeks  
**Doses:** 0, 25, 150, or 1000 mg/kg./day  
**Sex:** Males and females  
**Exposure period:** 4 weeks  
**Frequency of treatment:** Once daily, 7 days/week  
  
**Control group and treatment:** Concurrent vehicle control (corn oil)  
  
**Post exposure observation period:** None  
  
**Statistical methods:** Analysis of variance (Snedecor and Cochran, 1980) Kruskal-Wallis non-parametric analysis (Hollander and Wolfe, 1973) Fisher's Exact Probability test (Siegel 1956)  
  
**Test Conditions:** Groups of ten rats (5M:5F) were dosed orally by gavage once daily over a period of 28 days. Animals were approximately 41 days old on the first day of dosing. Animals were regularly monitored for any signs of ill health or reaction to treatment. Detailed functional observations were performed weekly, with additional functional observations performed during pretrial and week four. Animals were weighed daily to determine dose. Body weights and food consumption were recorded twice weekly. Blood and urine samples were collected during week four of the study. After four weeks of treatment animals were sacrificed and subjected to necropsy. A comprehensive list of organs were weighed and /or preserved (adrenal, brain, epididymis, eye, gastrointestinal tract including stomach, duodenum, jejunum, ileum, caecum, colon, rectum, heart, kidney, liver, lung, bone marrow, mesenteric lymph node, ovary, pituitary, prostate, sciatic nerve, spinal cord, spleen, submandibular lymph node, testis, thymus, thyroid with parathyroid, trachea, urinary bladder, uterus). Tissues from the controls and high dose animals were subjected to histological examination. Histology was also performed on the male kidneys from the lower doses.

## Results

**NOAEL (NOEL):** NOAEL = 1000 mg/kg/day (neurotoxicity)

**Actual dose received**

by dose level by sex if known: Actual doses for both sexes were 0, 25, 150, or 1000 mg/kg/day

Remarks: See Sec. 5.5.A for general toxicity results.

There was no evidence of neurotoxicity noted in animals treated at levels up to 1000 mg/kg/day.

**Reliability:** (1) Reliable without restrictions.

**Flag:** Key study for SIDS endpoint.

**References:** Clubb, S. (2000) AmoDrill 1000 4-Week Toxicity Study Including Neurotoxicity Screening in Rats with Administration by Gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE Scotland. Sponsor Amoco Corporation (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 1120-36-1, 1-Tetradecene

Remarks: Blend of three suppliers' 1-tetradecene, 99% purity

**Method**

Method/guideline: OECD 422 (See Sec. 5.5.B for general toxicity endpoints)

Test type: Combined repeated dose toxicity study with reproduction/developmental toxicity screening test

GLP: Yes

Year: 1995

Species: Rat

Strain: Sprague-Dawley

Route of Administration: Oral gavage

Duration of test: Up to 51 days; see Remarks

Doses: 0, 100, 500, or 1000 mg/kg b.w./day

Sex: Males and females

Exposure period: Up to 51 days, see Remarks

Frequency of treatment: Once daily

Control group and treatment: Concurrent vehicle control (corn oil)

Post exposure observation period: None

**Statistical methods:** Continuous data, including body weights, body weight gain, food consumption, clinical pathology data, organ weights, forelimb and hindlimb grip strength, landing footsplay and motor activity were analyzed by One-Way Analysis of Variance. If significance was detected, group by group comparisons were performed using Dunnett's test. All analyses utilized two-tailed tests for a minimum significance of 5% comparing the control group to the treated groups.

**Test Conditions:** This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Spraque Dawley rats. At study initiation, the males were 6 wks of age and weighed 159-220 g; the females were 8 wks of age and weighed 184-242 g (satellite) and 158-215 g (breeding). The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred.

Doses were selected based on the results of a 14-day rangefinding study. Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day, administered in a volume of 5 ml/kg. Animals were observed daily for signs of toxicity. Breeding females were All F0 males and females were subjected to gross necropsy when euthanized. Selected F0 males and all satellite females were evaluated for motor activity, clinical pathology, and functional observational battery before euthanasia. The liver, kidneys, testes/ovaries, adrenal glands, thymus, spleen, brain and heart of each animal were weighed. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues including nervous system tissues (brain, optic nerve, peripheral nerve, spinal cord) from five randomly selected males and satellite females from the control and high dose groups.

## **Results**

**NOAEL (NOEL):** 1000 mg/kg/day (neurotoxicity)

**Actual dose received  
by dose level by**

sex if known:	As administered. Analysis of dosing mixtures confirmed that mixtures were accurately prepared.
Remarks:	See Sec. 5.5.B for general toxicity results and Sections 5.9 A and B for reproductive and developmental toxicity results.  There were no test article-related differences in the functional observational battery and motor activity tests that would indicate neurotoxicity.
<b>Reliability:</b>	(1) Reliable without restrictions.
<b>Flag:</b>	Key study for SIDS endpoint.
<b>References:</b>	Daniel, E.M. (1995) Combined Repeated Dose Toxicity Study/Reproduction/Developmental Toxicity Screening Test in Rats with 1-Tetradecene. Conducted by Springborn Laboratories, Inc., Spencerville, Ohio, Study No. 3325.2 for the Chemical Manufacturers Association, Alpha Olefins Panel.
<b>Other:</b>	This study was included in the dossier for 1-tetradecene at SIAM 11.

### 5.11 Experience with Human Exposure

No data available

### 6.0 References

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