

201-15896D

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

ROBUST SUMMARIES DOSSIER

for

C8 MEMBERS

of the

HIGHER OLEFINS CATEGORY

Members containing C8 olefins:

CAS No. 25377-83-7, Octene
CAS No. 68526-54-5; Alkenes, C7-9, C8-Rich
CAS No. 68526-53-4; Alkenes, C6-8, C7-Rich*
CAS No. 68526-55-6; Alkenes, C8-10, C9-Rich*

* Addressed in the C7 and C9 dossiers.

Contains Robust Summaries for the Following Substances:

CAS No. 25377-83-7, Octene
CAS No. 111-66-0, 1-Octene
CAS No. 68526-54-5, Alkenes, C7-9, C8-Rich
C6-C8 Internal Olefins
CAS No. 111-67-1, 2-Octene
CAS No. 68526-55-6; Alkenes, C8-10, C9-Rich

Prepared by:

**American Chemistry Council
Higher Olefins Panel**

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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 (C₆ through C₅₄) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The C₆ – C₁₄ even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the C₆, C₇, C₈, C₉, C₁₀, C₁₂ and C₁₀₋₁₃ aliphatic linear and branched internal olefins and the C₁₆ and C₁₈ 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
Internal Olefins		
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	No data available	68526-53-4
Alkenes, C7-9, C8-rich	Linear	68526-54-5
Alkenes, C8-10, C9-rich	Linear	68526-55-6
Alkenes, C9-11, C10-rich	Linear	68526-56-7
Alkenes, C10-12, C11-rich	Linear	68526-57-8
Alkenes, C11-13, C12-rich	Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-0
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

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: Not applicable for Octene and Alkenes, C8-9, C8-rich as Octene is manufactured and marketed as a component of a blend and Alkenes C8-9, C8-rich is manufactured and marketed as a blend

1.2 Impurities

Remark: The compositions reported by manufacturers are shown below:

Octene	25377-83-7	C6-C8 internal olefin blend: Typical composition = 1.9% C5, 43.3% C6, 21.7% C7, 31.7% C8, 1.4% C9
Alkenes, C7-9, C8-rich	68526-54-5	Mostly linear, less than 5% branched. Typical composition: 1% C7 olefins, 89% C8 olefins, 10% C9 olefins.

1.3 Additives

None

1.4 Synonyms

Some synonyms are: Octene, Isomer(s)
Octylene
Octenes

1.5 Quantity

Remarks: Range of U.S. production volumes for 2002 submitted by Higher Olefin Panel members to Panel Manager: CAS No. 25377-83-7, Octene = 50-100 million pounds; CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich = 10-50 million pounds

Reference: American Chemistry Council's Higher Olefins Panel (2002)

1.6 Use Pattern

A. General Use Pattern

Type of Use:	Category:
(a) Main Industrial Use	Use in closed systems Chemical industry – chemicals used in synthesis Intermediate
Remarks:	Intermediate in the manufacture of low molecular weight fatty acids, mercaptans, plasticizer alcohols, surfactants
(b) Main Industrial Use	Non-dispersive use Chemical industry – chemicals used in synthesis Intermediate
Remarks:	Intermediate in the manufacture of low molecular weight fatty acids, mercaptans, plasticizer alcohols, surfactants
(c) Main Industrial Use	Use in closed systems Polymers industry Intermediate

Reference: American Chemistry Council's Higher Olefins Panel (2002)

B. Uses In Consumer Products

Not applicable

1.7 Sources of Exposure

Source:

Remarks: These products are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (including polymers). No non-intermediate applications have been identified. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. It is a common practice to use personal protective equipment. In the case of dermal exposures, protective gloves would be worn due to the mildly irritating properties of this class of chemicals (ACC Higher Olefins Panel). Results from modelled data suggest that on-site waste treatment processes are expected to remove these substances from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge (EPIWIN, 2000b). These substances are not on the US Toxic Release Inventory (TRI) list (NLM, 2003). These olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

Reference: American Chemistry Council's Higher Olefins Panel (2002)

1.8 Additional Information

A. Classification and Labelling

B. Occupational Exposure Limits

Exposure Limit Value

Type: None established
Value:

Short Term Exposure Limit Value

Value: None established

C. Options for Disposal

Remarks: Incineration, 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. 25377-83-7, Octene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point value in °C: -109°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: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Test Substance

Identity: CAS No. 25377-83-7, Octene

Method

Method/
guideline followed: Calculated value using the computer program EPIWIN version 3.10
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 program used structure for 1-octene.

Results

Melting point value in °C: -69.8°C

Reliability: (2) Reliable with restrictions. The result is 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 (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: C6-C8 Internal Olefins

Method

Method/guideline followed: ASTM D2386
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point value in °C: -50°C

Reliability: (4) Not assignable. These data were not reviewed for quality.

References: Shell Chemicals UK Ltd. Chester (cited in IUCLID)

D. Test Substance

Identity: 2-Octene

Method

Method/guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point value in °C: -100.2 to -87.7°C

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

References: Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-233.

E. Test Substance

Identity: 3-Octene

Method

Method/guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point value in °C: -126 to -110 °C

Reliability: (2) Reliable with restrictions. These data were not reviewed for quality.

References: Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-233.

F. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

**Method/
guideline followed:** Calculated value using 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. EPIWIN program used structure for 1-octene.

Results

**Melting point
value in °C:** -69.8°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. 25377-83-7, Octene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Boiling point
value in °C: 123°C
Pressure: 1013
Pressure unit: hPa

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: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Test Substance

Identity: CAS No. 25377-83-7, Octene or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/
guideline followed: Calculated value using MPBPWIN version 1.40, a subroutine of EPIWIN version 3.10
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). The program used the structure for 1-octene.

Results

Boiling point
value in °C: 118.13°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 (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: ASTM D68

GLP: No data

Year: No data

Test Conditions: No data

Results

Boiling point value: 74-120°C

Pressure: No data

Remarks: Upper value is for 90% distilled.

Reliability: (4) Not assignable. These data were not reviewed for quality.

References: Shell Chemicals UK Ltd. Chester (cited in IUCLID)

D. Test Substance

Identity: 2-Octene

Method

Method/guideline followed: No data

GLP: No data

Year: No data

Test Conditions: No data

Results

Boiling point value: 125 – 125.6°C

pressure: 1013

Pressure unit: hPa

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

References: Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-233.

E. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Boiling point value: 110 – 126°C
Pressure: No data

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

References: ExxonMobil (2004). Octene Datasheet. Unpublished data.

2.3 Density

A. Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: ISO 3675
GLP: No data

Test Conditions: No data

Results

Type: density
Value: ca. 700 kg/m³
Temperature (°C): 20°C

Reliability: (2) Reliable with restrictions. These data were not reviewed for quality.

Reference: Shell Chemicals UK Ltd. Chester (cited in IUCLID)

B. Test Substance

Identity: 2-Octene

Method

Method: No data

GLP: No data

Test Conditions: No data

Results

Type: density

Value: 0.7199 - 0.7243 g/cm³

Temperature (°C): 20°C

Reliability: (2) Reliable with restrictions. Reliable secondary source. These 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. 3-233.

C. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method: No data

GLP: No data

Test Conditions: No data

Results

Type: density

Value: 0.73 g/cm³

Temperature (°C): 20°C

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

Reference: ExxonMobil (2004) Octene Datasheet (unpublished data).

2.4 Vapour Pressure

A. Test Substance

Identity: CAS No. 25377-83-7, Octene or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/
guideline followed: Calculated value using MPBPWIN version 1.40, a subroutine of EPIWIN version 3.10

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 an experimental value for BP of 123 °C, cited in the EPIWIN database.

Results

Vapor Pressure

Value: 22 hPa

Temperature: 25°C

Remarks: Reported as 16.5 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 (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method/
guideline followed: No data

GLP: No data

Year: No data

Test Conditions: No data

Results

Vapor Pressure

Value: 23.2 hPa

Temperature: 25°C

Remarks: Reported as 17.4 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in EPIWIN.

Flag: Key study for SIDS endpoint

References: Yaws (1994); cited in EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

2.5 Partition Coefficient (log₁₀K_{ow})

A. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method: No data

GLP: No data

Year: No data

Test Conditions: No data

Results

Log K_{ow}: 4.57

Temperature (°C): No data

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

Reference: Hansch, C., A. Leo and D. Hoekman (1995) Exploring QSAR. Hydrophobic, Electronic, and Steric constants. ACS Professional Reference Book. Washing, DC: American Chemical Society.

EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: No data

GLP: No data

Year: No data

Test Conditions: No data

Results

Log Kow: 3.4 – 4.6

Reliability: (4) Not assignable. These data were not reviewed for quality.

References: Shell Chemicals UK Ltd. Chester, as cited in IUCLID

C. Test Substance

Identity: CAS No. 25377-83-7, Octene or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method: Calculated value using the computer program EPIWIN version 3.10, subroutine KOWWIN v 1.66

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). The program used the structure for 1-octene.

Results

Log Kow: 4.13

Temperature (°C): Not applicable

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

Reference: Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.
EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

2.6.1 Water Solubility (including *Dissociation Constant).

A. Test Substance

Identity: CAS No. 25377-83-7, Octene

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. Experimental Log Kow value of 4.57 from EPIWIN database used for calculation. Used experimental melting point of -109°C for correction.

Results

Value(mg/L) at
temperature (°C): 3.65 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.

B. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Value (mg/L)
at temperature (°C): 4.1 mg/L (25°C)

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

Flag: Key study for SIDS endpoint

References: Yalkowsky, S.H. and R.M. Dannenfelser (1992) AQUASOL dATABASE of Aqueous Solubility. Fifth ed. Tucson, AZ, University of Arizona, College of Pharmacy

EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

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. Experimental Log Kow value of 4.57 from EPIWIN database used for calculation. Used formula used when no melting point available.

Results

Value(mg/L) at
temperature (°C): 3.89 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)

Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: ISO 2719
GLP:

Test Conditions: No data

Results

Value (°C): -26 °C
Type of test: Closed cup

Reliability: (4) Not assignable. These data were not reviewed for quality.

Reference: Shell Chemicals UK Ltd. Chester (cited in IUCLID)

2.8 Auto Flammability (Solids/Gases)

No data available

2.9 Flammability

Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: No data
GLP: No data

Test Conditions: No data

Result: Highly flammable

Lower flammability limit: 0.8% in air
Upper flammability limit: 6.8% in air

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

Reference: Shell Chemical Company MSDS

2.10 Explosive Properties

No data available

2.11 Oxidising Properties

No data available

2.12 Oxidation-Reduction Potential

No data available

3. ENVIRONMENTAL FATE AND PATHWAYS**3.1 Stability****A. Photodegradation****(1) Test Substance**

Identity: CAS No. 25377-83-7, Octene; or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

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. 25377-83-7, Octene

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 and Howard (1993). Program used structure for 1-octene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser (type): OH
Rate Constant: 33.0041 E-12 cm³/molecule-sec
Degradation % after: 50% after 3.889 hrs (using a 12-hr day and avg. OH conc. of 1.5 E6 OH/cm³)

Sensitiser (type): Ozone
Rate Constant: 1.2 E-17 cm³/molecule-sec
Degradation % after: 50% after 22.920 hrs (using avg. ozone conc. of 7 E11 mol/cm³)

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 (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Stability in Water

Test Substance

Identity: CAS No. 25377-83-7, Octene; or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

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 (H₂O) 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 C8 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. 25377-83-7, Octene

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, 2000b)

Chemical assumptions:

Molecular weight: 112
Water solubility: 4.1 g/m³
Vapor pressure: 2320 Pa (25°C)
Log Kow: 4.57
Melting point: -109°C
Environment name: EQC Standard Environment

Half-life in air = 6.3 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

	Level I	Level III
Air	100%	7.4%
Water	<1%	69.2%
Soil	<1%	17.4%
Sediment	<1%	5.9%

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

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

Reliability: (2) Valid with restrictions: 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 (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.

B. Test Substance

Identity: CAS No. 25377-83-7, Octene

Method

Type: Volatilization from water

Remarks: Calculated using the computer program EPIWIN version 3.10, using a Henry's Law Constant of 0.627 atm-m³/mole (HENRYWIN experimental database) and EPIWIN default values

Results: Half-life from a model river: 1.082 hrs
Half-life from a model lake: 4.2 days

Reliability: (2) Valid with restrictions. Values are calculated.

References: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10 Syracuse Research Corporation, Syracuse, NY. USA.

3.3.2 Distribution

A. Test Substance

Identity: CAS No. 25377-83-7, Octene

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; program used chemical structure for 1-octene

Results

Value: Estimated Koc = 506.7

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

Reference: Meylan, W., P.H. Howard and R.S. Boethling (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-7

EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

B. Test Substance

Identity: CAS No. 25377-83-7, Octene

Method

Method: Henry's Law Constant calculated value using the computer program EPIWIN, HENRYWIN v 3.10

Test Conditions: Bond and Group estimates based on chemical structure, at 25°C;
VP/water solubility estimates based on EPIWIN values of VP = 16.5mm Hg and WS = 3.88 mg/L ; program used chemical structure for 1-octene

Results

Value: Bond estimate = 0.632 atm-m³/mole
Group estimate = 1.07 atm-m³/mole
VP/Wsol estimate = 0.667 atm-m³/mole

Reliability: (2) Reliable with restrictions. Values are calculated.

Reference: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

3.4 Aerobic Biodegradation

A. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline: OECD 301F, Ready Biodegradability, Manometric Respirometry Test

Type: Aerobic [X] Anaerobic []

GLP: Yes

Year: 1995

Contact time: 28 days

Inoculum: Domestic activated sludge

Test Conditions: Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, and calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material loading was approximately 32 mg/L. [Reason for

using 32 mg/L instead of 100 mg/L: Substances such as this test material typically have ThODs between 2 and 3 mg per mg substance. Thus, the test material concentration was adjusted for a target of 100 mg THOD/L] Sodium benzoate (positive control) concentration was approximately 44 mg/L. Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results: Approximately 29% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on day 17.

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

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	44.1, 28.6, 15.0	29.2
Na Benzoate	98.9, 95.5	97.2

* replicate data

Reliability: (2) Reliable with restrictions: The range in biodegradation values is not less than 20% as required in the OECD test guideline.

Flag: Key study for SIDS endpoint

Reference: Exxon Biomedical Sciences, Inc. (1997) Alkenes, C7-9, C8 Rich: Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119194A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

B. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method/guideline: 28-Day Ready Biodegradability, closed bottle Sturm, CO₂
Type: Aerobic [X] Anaerobic []
GLP: No
Year: 1985
Contact time: 28 days
Inoculum: *Pseudomonas fluorescens*

Test Conditions: Test medium was water. No other details available.

Results: 41-42% biodegradation after 28 days

Reliability: (4) Not assignable: The source of the report is reliable, but details of the test conditions and results are not available.

Reference: Adema, D.M.M., and Bakker, G.H. (1985) (unpublished report). [no further information is available]

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

C. Test Substance

Identity: CAS No. 25377-83-7, Octene

Method

Method/guideline: Estimated using the computer program EPIWIN v 3.10, BIOWIN v 4.00
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: Weeks
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)

3.5 BOD5, COD or ratio BOD5/COD

No data available

3.6 Bioaccumulation

Test Substance

Identity: CAS No. 25377-83-7, Octene

Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.14

Test Conditions: Based on chemical structure and a Log Kow of 4.57 (experimental data from EPIWIN database) using methods described by Meylan et al., 1999. Formula used to make BCF estimate: $\text{Log BCF} = 0.77 \text{ log Kow} - 0.70$ with no correction factor.

Results

Value: Estimated Log BCF = 2.819 (BCF = 659)

Reliability: (2) Reliable with restrictions. Value is 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 (2000a) Estimation Program Interface for Windows, version 3.10.
Syracuse Research Corporation, Syracuse, NY. USA.

3.7 Additional Information

A. Sewage Treatment

Test Substance

Identity: CAS No. 25377-83-7, Octene

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

Input values: MW = 112.22; Henry's LC = 0.627 atm-m³/mol; air-water partition coefficient = 25.6424; Log Kow = 4.57; biomass to water partition coefficient = 7431.51; temperature = 25°C

GLP: No
Test Medium: Secondary waste water treatment (water)
Test Type: Aerobic

Test Results: 99.70 % removed from wastewater treatment

Reference: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

4. ENVIRONMENTAL TOXICITY

4.1 Acute Toxicity to Fish

A. Test Substance

Identity: CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline: OECD 203
Test type: Semi-static Fish Acute Toxicity Test
GLP: Yes [X] No []
Year: 1995
Species/Strain: Rainbow Trout (*Oncorhynchus mykiss*)
Analytical Monitoring: Yes
Exposure period: 96 hours
Statistical methods: Trimmed Spearman-Kärber Method (Hamilton, M.A. et al. 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.)

Test Conditions: Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of <10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 2.6, 4.3, 7.2, 12, and 20 mg/L, which measured 0.2, 0.4, 0.7, 1.2, and 2.5 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions.

A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Water hardness was 174-178 mg/L as CaCO₃. Test temperature was 15C (sd = 0.09). Lighting was 578 to 580 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.5 to 10.2 mg/L for "new" solutions and 6.5 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.0 to 8.4 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

Results: 96-hour LL50 = 8.9 mg/L (95% CI 9.9 to 13.3 mg/L) based upon loading rates.
96-hour LC50 = 0.87 mg/L (95% CI 0.79 to 0.96 mg/L) based upon measured values of old and new solutions.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

<u>Loading Rate (mg/L)</u>	<u>Measured Conc. (mg/L)</u>	<u>Fish Total Mortality (@96 hrs)*</u>
Control	Control	0
2.6	0.2	0
4.3	0.4	0
7.2	0.7	1
12	1.2	12
20	2.5	12

* 12 fish added at test initiation

Reliability: (1) Reliable without restriction

Flag: Key study for SIDS endpoint

References: Exxon Biomedical Sciences, Inc. (1996) Alkenes, C7-9, C8 Rich: Fish, Acute Toxicity Test. Study #119158. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

B. Test Substance

Identity: CAS No. 111-67-1, 2-Octene (trans)

Method

Method/guideline: 96 hour semi-static toxicity test
Test type: semi-static
GLP: No
Year: 1985
Species/Strain: *Brachydanio rerio* (zebra fish)
Analytical Monitoring: No
Exposure period: 96 hr
Statistical methods: The LL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

Test Conditions: The test animals were 4-6 weeks old, 3 ± 1 cm, born and grown in the laboratory in fresh-water. Necessary amounts of test material were added to 2 L fresh water (pH ~8, hardness ~210 mg CaCO₃ per liter) in glass stoppered conical flasks and stirred for 4 hr before adding test animals (10/ flask). Test conditions: 24°C; no aeration, food, or replicate; test medium renewed daily. At none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. The target for oxygen concentration was 70% of the saturation level. The concentrations tested: 0, 3.2, 5.6, 10, 18, 32, and 56 mg/L (nominal).

Results: LL₅₀ (24 hr) = 15 mg/L
LL₅₀ (48 hr) = 13 mg/L
LL₅₀ (72 hr) = 8.0 mg/L
LL₅₀ (96 hr) = 7.5 mg/L

NOEC (96 hr) = 3.2 mg/L (nominal)

Remarks: Assessment of condition of test animals compared to the controls was by visual estimation. The oxygen concentrations of some of the test solutions were low, but it was assumed that this did not greatly influence the test results.

Reliability: (2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.

References: Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).

C. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method/guideline: 96 hour semi-static toxicity test
Test type: semi-static
GLP: No
Year: 1985

Species/Strain: *Brachydanio rerio* (zebra fish)
Analytical Monitoring: No
Exposure period: 96 hr
Statistical methods: The LL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

Test Conditions: The test animals were 4-6 weeks old, 3 ± 1 cm, born and grown in the laboratory in fresh-water. Necessary amounts of test material were added to 1 L fresh water (pH ~8, hardness ~210 mg CaCO₃ per liter) in glass stoppered conical flasks and stirred for 4 hr before adding test animals (10/ flask). Test conditions: 24°C; no aeration, food, or replicate; test medium renewed daily. At none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. During the test, the oxygen concentration was >70% of the saturation level. The concentrations tested: 0, 3.2, 10, and 32 mg/L (nominal).

Results: LL₅₀ (24 hr) = >3.2 <10 mg/L
LL₅₀ (48 hr) = >3.2 <10 mg/L
LL₅₀ (72 hr) = >3.2 <10 mg/L
LL₅₀ (96 hr) = >3.2 <10 mg/L (estimated to be about 6 mg/L)
NOEC (96 hr) = 3.2 mg/L (nominal)

Remarks: Assessment of condition of test animals compared to the controls was by visual estimation.

Reliability: (2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.

References: Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).

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

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

A. Test Substance

Identity: CAS No. 111-67-1, 2-Octene (trans)

Method

Method/guideline: 48-hr static toxicity test
Test type: Static
GLP: No
Year: 1985

Analytical Monitoring: No
Species/Strain: *Daphnia magna*
Exposure period: 48 hrs
Statistical methods: The EL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

Test Conditions: Test media were prepared by adding test material to 500 ml of fresh water (pH ~8, hardness ~210 mg CaCO₃ per liter) in a glass-stoppered conical flask and stirring for 4 hr before adding test animals (25/ flask). Test conditions: 20 °C; no aeration, food, replicate or media renewal. The test animals were less than 24 hr old at the start of the test, from a laboratory culture in standard fresh water. At none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. During the test, the oxygen concentration was >70% of the saturation level. The concentrations tested: 0, 3.2, 10, and 32 mg/L (nominal).

Results: EL₅₀ (48 hr) = >3.2<10 mg/L (estimated to be about 6);
NOEC (48 hr) = 3.2 mg/L (nominal)

Remarks: Assessment of condition of test animals compared to controls was by visual estimation.

Reliability: (2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.

Flag: Key study for SIDS endpoint

References: Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).

B. Test Substance

Identity: CAS No. 111-66-0, 1-Octene

Method

Method/guideline: 48-hr static toxicity test

Test type: Static

GLP: No

Year: 1985

Analytical Monitoring: No

Species/Strain: *Daphnia magna*

Exposure period: 48 hrs

Statistical methods: The EL50 values were calculated by means of a parametric model developed by Kooijman [Kooijman, S.A.L.M. (1981) Parametric analyses of mortality rates in bioassays. Water Res. 15:105-119.]

Test Conditions:	Test media were prepared by adding test material to 500 ml of fresh water (pH ~8, hardness ~210 mg CaCO ₃ per liter) in a glass-stoppered conical flask and stirring for 4 hr before adding test animals (25/ flask). Test conditions: 20 °C; no aeration, food, replicate or media renewal. The test animals were less than 24 hr old at the start of the test, from a laboratory culture in standard fresh water. At none of the dose levels was test substance visible during the test period. pH and oxygen were monitored. During the test, the oxygen concentration was >70% of the saturation level. The concentrations tested: 0, 1.0, 3.2, and 10 mg/L (nominal).
Results:	EL ₅₀ (48 hr) = >3.2<10 mg/L (estimated to be about 6); NOEC (48 hr) = 3.2 mg/L (nominal)
Remarks:	Assessment of condition of test animals compared to controls was by visual estimation.
Reliability:	(2) Reliable with restrictions. Study does not totally comply with current testing guidelines. No chemical analyses were performed.
References:	Adema, D.M.M. and Bakker, G.H. (1985) Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague (unpublished report).
Flag:	Key study for SIDS endpoint
Other:	This study was included in the dossier for 1-octene at SIAM 11. Additional information has been added.

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

No data available.

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

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 8×10^{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 and 1-tetradecene at SIAM 11. Additional information has been added.

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

Test Substance: CAS No. 25377-83-7, Octene ; or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method/Guideline:

Type (test type): 30-day Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Fish

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 4.13, which was estimated by EPIWIN using the structure for 1-octene.

Results:

Units/Value: Estimated 30-day ChV = 150 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: 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.

B. Chronic Toxicity to Aquatic Invertebrates

Test Substance: CAS No. 25377-83-7, Octene ; or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method/Guideline:

Type (test type): 16-day EC50 value calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: *Daphnia magna*

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 4.13, which was estimated by EPIWIN using the structure for 1-octene.

Results:

Units/Value: Estimated 16-day EC50 = 134 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: 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.

4.6 Toxicity to Terrestrial Organisms

A. Toxicity to Terrestrial Plants.

Test Substance: CAS No. 25377-83-7, Octene ; or CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method/Guideline:

Type (test type): 96-hr Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Green algae

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 4.13, which was estimated by EPIWIN using the structure for 1-octene.

Results:

Units/Value: Estimated 96-hr ChV = 249 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: 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.

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

4.9 Additional Information

No data available

5. MAMMALIAN TOXICITY

5.1 Toxicokinetics, Metabolism and Distribution

A. Test Substance: CAS No. 111-66-0, 1-Octene; CAS No. 14850-23-8, trans-n-4-Octene; CAS No. 816-79-5, 3-Ethyl-2-Pentene (tested individually)

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

Method: Homogenized rat liver was incubated with olefins and metabolites were quantified using gas-liquid and thin layer cochromatography. Various experiments were conducted with and without NADPH and epoxide hydrolase inhibitors.

Test Conditions: Livers of male Sprague-Dawley rats, weighing 180-200 g were homogenized at 4°C in 2 volumes of isotonic KCl. For all experiments, the aliquots were equivalent to 2 g of liver. For quantification of metabolites, the reaction mixture was extracted with ether, the ether layer was removed and evaporated, the residue was dissolved in acetone and aliquots were analyzed in a model 5000 Barber-Colman gas chromatograph equipped with an ionization detector. With each olefin, the identities of the epoxide and glycol metabolites were checked by both gas-liquid and thin layer cochromatography.

Enzymatic oxidation of olefins experiments: Mixtures of 10 μ moles of olefin dissolved in ethanol, NADPH-enriched 9000 x g supernatant of 2 g liver and standard cofactors and phosphate buffer were incubated for 60 minutes at 37°C.

Effect of epoxide hydrolase inhibitor on metabolism of n-1-octene: 10 μ moles olefin in ethanol added to the incubation mixture described above. The medium contained the NADPH-generating system and the epoxide hydrolase inhibitor (2×10^{-2} M 4,5-epoxy-n-octane). Incubation time was 30 min.

Effect of the epoxide metabolite 1,2-epoxy-n-octane on the metabolism of n-4-octene: n-4-octene was incubated with 20 mM 1,2-epoxy-n-octane under the conditions described.

Results: In the presence of rat liver microsomes and NADPH, n-1-octene, n-4-octene and 3-ethyl-2-pentene were converted to the glycols with no trace of epoxide. The relative yields of the glycols from 10 μ moles of the olefins (11.3%, 4.0%, 0.12%) indicate that increasing substitution of the ethylenic moiety by alkyl groups decreases the rate of the reaction. In the presence of 4,5-epoxy-n-octane, the product from 10 μ moles n-1-octene contained both 1,2-epoxy-n-octane (0.40 μ moles) and n-octane-1,2-diol (0.23 μ moles), whereas in the absence of the inhibitor, only the glycol (0.64 μ moles) could be detected. Thus, the inhibition of glycol formation was 64%. In the presence of 1,2-epoxy-n-octane, the substrate n-4-octene produced the epoxide but not the glycol. The quantity of 4,5-epoxy-n-octane produced was approximately equivalent to the amount of glycol formed in the absence of the inhibitor. The authors concluded that it is likely that the biological conversion of the alkenes proceeds through epoxides.

Reliability: (1) Reliable without restrictions

Reference: Maynert, E.W., Foreman, R.L., and Watabe, T. (1970) Epoxides as obligatory intermediates in the metabolism of olefins to glycols. J. Biological Chemistry 245(20): 5324-5238.

Other: This study was cited in the dossier for 1-octene at SIAM 11.

B. Test Substance: CAS No. 111-66-0, 1-Octene

Method

Test Type: In vivo
GLP No data available
Year 1995

Method: Some olefins have been shown to be metabolized to epoxides. For example, ethylene and propylene have been shown to be metabolized to their corresponding oxides by the presence in animals of the

corresponding hemoglobin and DNA adducts. Absorption, distribution, elimination and hemoglobin and DNA adduct formation were studied in the rat after inhalation of individual C₂ - C₈ 1-alkenes [including 1-octene] at 300 ppm, 12 hr /day for 3 consecutive days. Concentrations of olefins were measured in blood, lung, brain, liver, kidney and perirenal fat immediately after each exposure and 12 h after the third exposure.

Results:

Concentrations of olefins reached steady state levels after the first 12 hr of exposure, and the concentrations 12 hr after the last exposure were generally low, except in the fat. Concentrations of 1-alkenes in blood and tissues increased with increasing number of carbon atoms. In contrast, levels of hemoglobin and DNA adducts decreased with increasing number of carbon atoms. The decrease was most pronounced from C₂ to C₃.

Concentrations of individual 1-alkenes after the third daily 12 hr exposure to 300 ppm and concentrations in fat 12 hr after the third exposure (n=4). All concentrations are in μmol/kg; nd = not detectable (detection limits not provided)

Chemical	Blood	Liver	Lung	Brain	Kidneys	Fat	Fat 12 hr after 3 rd exposure
Ethene	0.3	0.4	2.3	0.7	0.7	7	nd
Propene	1.1	0.3	2.9	1.7	1.8	36	nd
1-Butene	1.9	0.8	4.9	3.0	5.7	70	0.3
1-Pentene	8.6	51.6	31.4	41.0	105.7	368	19
1-Hexene	18.2	66.8	59.7	59.7	188.0	1031	77
1-Heptene	37.0	138.3	85.6	109.3	269.3	2598	293
1-Octene	60.1	443.7	202.4	270.0	385.1	4621	943

Remarks:

The increased retention in fat of 1-alkenes with higher carbon numbers is presumably a function of their increased lipophilicity, and decreased likelihood to be exhaled unchanged, compared to the lower volatile 1-alkenes. Since unchanged 1-alkenes are not considered to be toxic, and because tissue levels rapidly cleared after exposure ceased, this concentration, especially in fat tissues, is unlikely to have any biological effect. An implication of the metabolic formation of an epoxide, as determined by hemoglobin and DNA adducts, is that the 1-alkenes are likely to be genotoxic. However ethylene, which formed these adducts to a much greater extent than the higher homologs, has been specifically investigated in lifetime animal cancer bioassays at concentrations up to 3000 ppm, and determined to be negative [Hamm, T.E. Jr., Guest, D, and Dent, J.G. (1984) *Fundam. Appl. Toxicol.* 4(3 Pt 1):473-8]. It is highly unlikely that the higher homologs, including 1-octene, will be genotoxic or carcinogenic under these conditions.

Reliability:

(1) Reliable without restrictions.

Reference: Eide, I., R. Hagerman, K. Zahlsen, E. Tareke, M. Tornquist, R. Kumar, P. Vodicka and K. Hemminki (1995) Uptake, distribution, and formation of hemoglobin and DNA adducts after inhalation of C2-C8 1-alkenes [olefins] in the rat. *Carcinogenesis*. 16, 1603 - 1609.

Other: This study was included in the dossier for 1-hexene at SIAM 11. As the study also included 1-octene, the summary is included in this dossier. Additional information has been added.

C. Test Substance: CAS No. 111-66-0, 1-Octene, >99%; CAS No. 124-11-8, 1-Nonene, >99%; CAS No. 872-05-9, 1-Decene, >98% (tested individually)

Method Non-standard
Test Type in-vivo
GLP No data
Year No data

Method: Animals were exposed via inhalation to individual hydrocarbons in 6 separate experiments with equal design except for the choice of test substance. Animals were killed by decapitation, and blood and organ samples were obtained within 3 minutes after removal of an animal from the chamber. Food and water were available *ad libitum* except during exposure. Dynamic exposure of the animals was performed in 0.7 m³ steel chambers. Temperature and humidity were kept within 23±1°C and 70±20% RH, respectively. The aimed concentration of 100 ppm was maintained by mixing a controlled stream of air saturated with the test substance under a constant temperature and flow with the main stream of dust filtered air (5 m³/hr) before entering at the top of the chamber. The concentration of hydrocarbons in the chambers was monitored by on-line gas chromatography at 15 minute intervals. The concentration of hydrocarbons in tissues was determined by headspace gas chromatography. Two ml of blood or organ homogenate (or 0.25 g perirenal fat tissue) was equilibrated in 15 ml headspace vials for 1 hr at 37 or 60 °C together with calibration samples and blanks. 0.5 ml was taken from the headspace by prewarmed gas tight syringe and injected into a Shimadzu GC 9A gas chromatograph (FID). Separation was performed on a 2 m x 1/8" stainless steel column packed with GP 10% SP-2100 on Supelcoport 100/120 mesh with nitrogen as carrier gas. In blood, the calibration curves covered a range from 0.5 – 100 µmol/kg, in organs from 1 – 500 µmol/kg and in fat from 5 – 10000 µmol/kg. In blood and organs, the detection limits generally were within the range from 0.1 to 1 µmol/kg; in fat from 1 to 10 µmol/kg.

Test Conditions:

Species: Rat

Strain: Sprague-Dawley

Sex: Male

Age: No data

Bodyweight: 150 – 200 g at start of each experiment

Number of Animals: 4 per exposure

Route: Inhalation

Dose(s) used: 100 ppm for 3 days, 12 hr/day

Statistical Methods: None reported

Actual Dose(s): For the 3 days exposure period, the mean chamber concentration was 99.3 ppm

Body Fluids Sampled: Blood sampled at days 1, 2, and 3, immediately after exposure and 12 hr after exposure on day 3

Tissues Sampled: Brain, liver, kidney, fat; sampled at days 1, 2, and 3, immediately after exposure and 12 hr after exposure on day 3

Results: No systematic increase or decrease in biological concentrations was observed during the exposure period except for fat. With the exception for the kidney, the concentration increased with increasing number of carbon atoms within each structure group. The organ concentrations generally exceeded blood by factors ranging from 3 to 10. The C9 and C10 1-alkenes showed an increased accumulation in fat during the 3 days exposure period, in contrast to the C8 1-alkene, where a saturation seemed to occur. In fat, the concentrations of all hydrocarbons were 4-20 times the concentrations found in other organs. The 1-alkenes demonstrated high concentrations in fat 12 hr after exposure. After the recovery period, these concentrations were 31, 46, and 66% for C8, C9 and C10 1-alkenes, respectively, of the concentrations on day 3.

Concentrations of individual 1-alkenes after the third daily 12 hr exposure to 100 ppm and after 12 hr recovery (n=4)^a

	1-Octene		1-Nonene		1-Decene	
	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery
Blood	12.4	0.1	15.9	0.4	16.4	0.7
Brain	69.7	0.5	116.3	2.7	138.1	6.3
Liver	78.9	nd	130.4	1.1	192.8	4.0
Kidney	139.3	0.9	146.7	4.6	162.0	9.3
Fat	720	226	2068	953	2986	1971

^a All concentrations are in $\mu\text{mol/kg}$; nd = not detectable (limit of detection varied between substances and organs: in blood and organs generally within range from 0.1 – 1 $\mu\text{mol/kg}$; in fat from 5 – 10 $\mu\text{mol/kg}$)

Reliability: (1) Reliable without restrictions

Reference: Zahlse, K., I. Eide, A.M. Nilsen and O.G. Nilsen (1993) Inhalation kinetics of C8 to C10 1-alkenes and iso-alkanes in the rat after repeated exposures. *Pharmacology & Toxicology* 73 :163-168

D. Test Substance: CAS No. 592-76-7, 1-Heptene ; CAS No. 2216-38-8, 2-Nonene; CAS No. 592-47-2, 3-Hexene; CAS No. 16746-85-3, 4-Ethyl-1-Hexene; CAS No. 15870-10-7, 2-Methyl-1-Heptene; CAS No. 3404-77-13, 3-dimethyl-1-hexene; 3-methyl-1-octene (tested individually)

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

Test Conditions: In-vitro: Incubation of hepatic microsomes from rats in the presence of alkenes and NADPH with analysis for presence of cytochrome P-450.

In-vivo: Phenobarbital-treated rats were injected i.p. with 1-heptene, *cis* and *trans* 2-nonen, 4-ethyl-1-hexene, and 3-methyl-1-octene at a dose of 400 $\mu\text{l/kg}$. Four hrs after treatment, animals were sacrificed and livers were analyzed for the presence of abnormal hepatic pigments. These pigments have been shown to be porphyrins derived from the prosthetic heme moiety of inactivated P-450 enzymes.

Results: *In vitro*: Hepatic microsomal cytochrome P-450 was destroyed *in vitro*, in the presence of NADPH, by 4-ethyl-1-hexene, 3-methyl-1-octene, and 1-heptene. The *cis*- and *trans*-2-nonenes exhibited marginal destructive activity (10% loss after 30 minutes). No significant cytochrome P-450 loss was observed after incubation with 2-methyl-1-heptene, 3,3-

dimethyl-1-hexene or 3-hexene, suggesting that steric and electronic factors can suppress the destructive interaction. The epoxides of 3 of the terminal olefin substrates were synthesized and shown not to intervene in destruction of the enzyme by the parent olefins.

In vivo: Hepatic green pigments were formed after administration of 4-ethyl-1-hexene, 3-methyl-1-octene and 1-heptene, indicating destruction of the P-450 enzyme. The cis- and trans-2-nonenones produced no abnormal pigments.

Reliability: (1) Reliable without restrictions

Reference: Ortiz de Montellano, P.R., and Mico, G.A. (1980) Destruction of cytochrome P-450 by ethylene and other olefins. *Mol. Pharmacol.* 18(1)128-135.

E. Test Substance: n-1-Octene, n-4-Octene, and 3-Ethyl-2-Pentene (tested individually)

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

Method: n-1-Octene (A), n-4-Octene (B), and 3-Ethyl-2-Pentene (C) and the corresponding epoxides and glycols were studied systematically in an attempt to detect epoxide intermediates in the biotransformation of olefins.

Test Conditions:

Results: In the presence of rat liver microsomes and TPNH, all 3 olefins were converted to the glycols with no trace of epoxides. Treatment of B ($1.6 \times 10^{-3}M$) with microsomes and TPNH in the presence of the A-epoxide ($2 \times 10^{-2}M$) yielded B-epoxide without B-glycol. In contrast, A in the presence of B-epoxide yielded approximately equal amounts of A-epoxide and A-glycol. C-epoxide was ineffective in inhibiting the hydrolase. The experiment involving A-epoxide as a blocking agent indicates that epoxides are obligatory intermediates in the conversion of olefins to glycols.

Reliability: (2) Reliable with restrictions: report was an abstract with limited data.

Reference: Watabe, T. and E.W. Maynert (1968) Role of epoxides in the metabolism of olefins. *Pharmacologist* V10(1) :203

5.2 Acute Toxicity

A. Acute oral toxicity

(1) Test Substance

Identity (purity): CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline: NA
Type (*test type*): LD50
GLP: Pre-GLP
Year: 1975
Species/Strain: Albino Rat
Sex: Males
No. of animals per sex per dose: 10

Vehicle: NA
Route of administration: Oral gavage

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. Age of the test animals was not reported. Body weights ranged from 166 to 206g at initiation of the study and from 220 to 260g on Day 7. A single dose of undiluted test material (5,000 mg/kg) was administered to male rats (not fasted). Individual body weights were recorded on Day 0 and Day 7. Gross necropsy examinations were performed on all animals that died or were killed. The statistics used to analyze the data were not reported.

Results:

Value: LD50 > 5000 mg/kg
Number of deaths at each dose level: There were no deaths

Remarks: Hypoactivity and diarrhea were noted within 6-22 hours post-oral administration and subsided by the second post-oral exposure day. There were no significant findings observed during the gross necropsy examination. Under the conditions of this study, Alkenes, C7-9, C8 Rich have a low order of acute oral toxicity.

Reliability: (1) Reliable without restrictions, comparable to a guideline study

Flag: Key study for SIDS endpoint.

References: Exxon Research and Engineering Company (1975) Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 111-66-0, 1-Octene (NEODENE 8 Alpha Olefin)

Method

Method/guideline: Not specified
Type (*test type*): LD50
GLP: Yes [X] No []
Year: 1983
Species/Strain: Rat/Fisher 344
Sex: Males and females
No. of animals per
sex per dose: 5 in first test and 10 in confirmation group

Vehicle: None
Route of
administration: oral gavage

Test Conditions: Undiluted NEODENE 8 Alpha Olefin caused no deaths at volumes of 1.0, 2.5, and 5 ml/kg body weight. The confirmation dose of 5.0 ml/kg given to 10 animals (5 female, 5 male) caused no deaths. Statistical analysis of body weights included calculation of the mean and standard error. Determination of the significance of body weight changes on days 7 and 14 compared to controls was made using an independent T-test. The lethal dose was not calculated but was found to be greater than 5.0 ml/kg body weight in the rat.

Results:

Value: LD50 > 5 ml/kg; >5 g/kg
Number of deaths
at each dose level: No deaths at 5 ml/kg

Remarks: Clinical signs of toxicity occurred at the 5.0 ml/kg dose level. Test animals generally recovered in 1 to 4 days. Prominent clinical signs of toxicity included hunched posture, unsteady stance, tip-toe gait, and hypoactivity. Less prominent effects included stool with mucus and polyruia. All remarkable observations at necropsy are considered to be incidental findings and not related to treatment with octene. Observations included clear discharge from the left eye and incomplete diaphragmatic hernia in one animal.

Reliability: (1) Reliable without restrictions: Deviations were limited to environmental conditions which did not effect the outcome or the validity of the study.

Flag: Key study for SIDS endpoint

References: Shell Development Company, Westhollow Research Center (1983)
Acute Oral Toxicity of NEODENE 8 Alpha Olefin in the Rat.
(unpublished report).

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

B. Acute inhalation toxicity

(1) Test Substance

Identity (purity): CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline: NA
Type (test type): Inhalation LC50
GLP: Pre-GLP
Year: 1977
Species/Strain: Albino Mice, Rats, and Guinea Pigs
Sex: Males
No. of animals per sex: 10/species

Vehicle: None
Route of administration: Inhalation (vapor)

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. Age of animals was not reported. Animals were given single doses of test substance vapor at a concentration of 31.67 mg/L (6900 ppm) for 6 h. The exposure was conducted in a 100-liter glass and stainless steel chamber. The compound was placed in a 2000 ml three-necked flask, pre-weighed and mounted outside the chamber. Air was bubbled through the test material at 5 L/min and was then combined with an additional airflow of 10 L/min to produce a total flow rate through the chamber of 15 L/min. Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group.

All animals were observed for signs of toxicity, abnormal behavior, and mortality during the exposure period and for 14 days after the exposure. Necropsies were performed on all surviving animals and any animals that died during the exposure or post-exposure observation period. Statistics used to evaluate data were not reported.

Results:

Value: LC50 > 31.7 mg/L (6900 ppm) for 6 h for rats and mice
LC50 <31.7 mg/L (6900 ppm) for 6 h for guinea pigs

Number of deaths
at each dose level:

There were no deaths in the air-exposed animals. In the treated animals, six guinea pigs and three rats died during the exposure period. No mice died during the study. One guinea pig died on Day 1 of the recovery period.

Remarks:

All animals showed compound awareness 1 minute after exposure began and became increasingly agitated during the first 35 minutes of exposure. After 100 minutes, some animals were experiencing tremors and convulsions. Necropsy examination indicated dark red coloration of the lungs of 15 animals (3 rats, 4 mice, and 8 guinea pigs). Six guinea pigs had liver discolorations. Five guinea pigs showed pale kidney color also. One guinea pig that died showed a large amount of blood in the heart. Fifteen animals (7 rats, 6 mice, and 2 guinea pigs) showed no gross lesions. Under conditions of this study, Alkenes, C7-9, C8 Rich have a low order of acute inhalation toxicity in rats.

Reliability:

(1) Reliable without restrictions; comparable to a guideline study.

Flag:

Key study for SIDS endpoint

References:

Exxon Corporation. (1977) Acute Inhalation Toxicity - Rats, mice and guinea pigs (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 111-66-0, 1-octene (Ethyl Corporation)

Method

Method/guideline: Not specified
Type (*test type*): LC50
GLP: Yes [] No [X]
Year: 1973
Species/Strain: Rat/Sprague-Dawley
Sex: Males
No. of animals per sex per dose: 10
Vehicle: None
Route of administration: Inhalation (vapor)

Test Conditions:	Six groups of 10 male rats (200-300 g, age not reported) each were exposed to concentrations ranging from 28.0 – 53.6 mg/L (6,050 to 11,580 ppm) for 4 hours. The exposure atmosphere was generated by bubbling air through 1-octene liquid and mixing the effluent vapor with varying amounts of air before entering the exposure chamber.
Results:	
Value:	LC50: 36.9 mg/L (nominal) (8,050 ppm) (4 hr)
Number of deaths at each dose level:	<u>Mortality per group at nominal concentrations:</u> Gp. I (28.0 mg/L) = 0/10 Gp. II (31.1 mg/L) = 2/10 Gp. III (36.0 mg/L) = 5/10 Gp. IV (40.5 mg/L) = 6/10 Gp. V (48.4 mg/L) = 9/10 Gp. VI (53.6 mg/L) = 10/10
Remarks:	A preliminary one hour study at the saturated vapor limit (87.5 mg/L nominal concentration; 19,110 ppm) caused deaths in 9 of 10 male Sprague Dawley rats. Necropsy revealed hemorrhagic lungs, very pale kidneys and nutmeg livers. The one surviving animal was observed 14 days after exposure, sacrificed and autopsied. There were no signs of gross pathological changes 14 days after exposure. In the main study, all deaths occurred within the exposure period. Also during exposure, animals exhibited labored breathing, erythema of exposed skin, and body tremors. Surviving animals began immediate recovery upon exposure to fresh air. Necropsy at the end of the 14-day observation period did not reveal any significant pathological changes.
Reliability:	(2) Reliable with restrictions: Incomplete reporting of experimental details including age of animals at initiation, body weight changes and incidence and severity of clinical observations. Study relied on nominal concentrations rather than measured chamber concentrations.
Flag:	Key study for SIDS endpoint
References:	Ethyl Corporation (1973) Report on the Acute Toxicity of Alpha Olefin C8, conducted by Tulane University School of Medicine (unpublished report).
Other:	This study was included in the dossier for 1-octene at SIAM 11. Additional information has been added.

C. Acute dermal toxicity

(1) Test Substance

Identity (purity): CAS No. 68526-54-5; Alkenes, C7-9, C8 Rich

Method

Method/guideline: NA
Type (*test type*): LD50
GLP: Pre-GLP
Year: 1975
Species/Strain: Albino rabbits
Sex: Males and females
No. of animals
per sex per dose: 2

Vehicle: NA
Route of
administration: Dermal

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. A single dermal application of the test material was made to two groups of four rabbits at doses of 200 and 3,160 mg/kg. The test material was applied to abraded skin. The duration of exposure was 24 hours. Individual body weights were recorded on Days 0, 7 and 14. Gross necropsies were performed at the end of the experiment. Age of test animals and the statistics used to evaluate the data were not reported.

Results:

Value: LD50 > 3160 mg/kg
Number of deaths
at each dose level: No mortalities were observed at any dose tested.

Remarks: There were no mortalities at any dosage level tested. Thus, the LD₅₀ in albino rabbits is greater than the highest dose tested. Signs of erythema, mild to moderate edema and second degree burns were observed at 24 hours at both doses. At 7 and 14 days, focal escharosis was observed at the low dose. At the high dose, escharosis, fissuring, hemorrhaging, and wrinkling were observed at 7 days and escharosis was observed at 14 days. Necropsy examination revealed emaciation and depletion of fat stores in one male rabbit in the low dose group. No other gross pathologic alterations were observed. Under the conditions of this study, Alkenes, C7-9, C8 rich have a low order of acute dermal toxicity.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Exxon Research and Engineering Company (1975) Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 111-66-0, 1-Octene (NEODENE 8 Alpha Olefin)

Method

Method/guideline: Not specified
Type (test type): LD50
GLP: No
Year: 1983
Species/Strain: Albino rabbits/New Zealand White
Sex: Males and females
No. of animals per sex per dose: 8

Vehicle: None
Route of administration: Dermal

Test Conditions: Groups of 16 (8 M, 8 F) rabbits were dosed with 2 ml/kg undiluted test material (NEODOL-8) under an occlusive dressing for 24 hours. Age of animals was not specified.

Results:

Value: LD50 > 1.43 g/kg
Number of deaths at each dose level: No mortalities were observed.

Remarks: There were no deaths or major gross pathological changes. Mild to moderate skin irritation was present at the site of application, after patch removal, which became less pronounced (but not fully reversed) over 14 days.

Original study indicated a Dermal LD₅₀ >2 ml/kg/bw however US EPA review prior to SIAM 11 indicated that the LD₅₀ should be changed to reflect 1.43 g/kg in a memo dated 8/14/96. As a result the LD₅₀ for this study was changed from > 2 ml/kg/bw to 1.43 g/kg. The only remarkable necropsy findings were those related to the exposure site (white crusty material on skin and fur, alopecia, abrasions, erosion, and focal cutaneous firmness in one animal).

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Shell Development Company, Westhollow Research Center (1983) Acute Dermal Toxicity of NEODENE 8 Alpha Olefin in the Rabbit. (unpublished report).

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

D. Acute toxicity, other routes

No data available

5.3 Corrosiveness/Irritation

A. Skin Irritation/Corrosion

(1) **Test Substance:** CAS No. 111-66-0, 1-Octene (NEODENE 8 alpha olefins)

pH: Not applicable

Method: OECD 404

Test Type: in vivo

GLP: Yes

Year: 1992

Test Conditions

Species: Rabbits

Strain: New Zealand White

Cell type:

Sex: Male and female

Number of animals per sex per dose: 3 male, 3 female

Total dose: 0.5 ml

Vehicle: None

Exposure time period: 4 hrs

Grading scale: Draize

Method Remarks: Neat substance was applied to shaved, intact dorsal skin. Draize scoring was made at 4, 24, 48 and 72 hour contact for erythema and edema. (Further scoring was conducted at 7days)

Results: Primary Irritation Index score 4.2 (max. 8.0). Mean score for 24+48+72 hour was 2.28 for erythema; maximum single score was 1.83 for edema. Effects disappeared within 14 days.

Reliability: (1) Reliable without restrictions

Reference: Morris, TD, Primary skin irritation study on rabbits of Neodene 8 alpha olefin. Report ref: 91-8385-21 from Hill Top Biolabs Inc. to Shell Oil Company (unpublished report).

(2) **Test Substance:** CAS No. 111-66-0, 1-Octene (GULFTENE 8 Alpha Olefin)

pH: Not applicable

Method: OECD 404

Test Type: in vivo

GLP: No

Year: 1996

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 hr

Grading scale: Draize

Method Remarks: At the start of the study, the animals weighed 2.45 to 2.70 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabrased 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 and slight to severe edema which cleared by day 7. Other dermal reactions noted were desquamation and crust formation which persisted to day 14, but were considered to be reversible effects. The Draize primary irritation index was 3.42. The mean 24-72 hr scores for erythema and edema were 1.9 and 1.1 respectively.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 8, Report 703/076. Conducted by Safepharm Laboratories Ltd. for Chevron Chemical Company (unpublished report).

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

(3) **Test Substance**

Identity (purity): CAS No. 68526-54-5; Alkenes, C7-9, C8 rich

Method

Method/guideline: NA
Type (*test type*): Dermal irritation
GLP: Pre-GLP
Year: 1975
Species/Strain: Albino rabbits
Sex: Males and females
No. of animals per sex per dose: 2

Vehicle: NA
Route of administration: Dermal

Test Conditions: A single dermal application of the test material was made to two groups of four rabbits at doses of 200 and 3,160 mg/kg. The test material was applied to abraded skin. The duration of exposure was 24 hours. Individual body weights were recorded on Days 0, 7 and 14. Gross necropsies were performed at the end of the experiment. Age of the test animals and the statistics used to evaluate the data were not reported.

Results:

Number of deaths at each dose level: No mortalities were observed at any dose tested.

Remarks: Signs of erythema, mild to moderate edema and second degree burns were observed at 24 hours at both doses. At 7 and 14

days, focal escharosis was observed at the low dose. At the high dose, escharosis, fissuring, hemorrhaging, and wrinkling were observed at 7 days and escharosis was observed at 14 days. Necropsy examination revealed emaciation and depletion of fat stores in one male rabbit in the low dose group. No other gross pathologic alterations were observed.

Reliability: (1) Reliable without restrictions; however, exposure was more severe than recommended by current testing guidelines (i.e., current guidelines recommend exposing non-abraded skin and exposure durations of 4 rather than 24 hours)

References: Exxon Research and Engineering Company (1975) Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study (unpublished report).

B. Eye Irritation/Corrosion

(1) **Test Substance:** CAS No. 111-66-0, 1-Octene (NEODENE 8 alpha olefin)

pH: Not applicable

Method: U.S. FHSA method

Test Type: in vivo

GLP: Yes

Year: 1983

Test Conditions

Species: Albino rabbits

Strain: New Zealand White

Cell type:

Sex: 3 male and 3 female; additional 3 males washed

Number of animals per dose: 9 (6 unwashed and 3 washed)

Dose(s) used: 0.1 ml

Vehicle: None

Observation period: 7 days

Scoring method used: Draize scoring at 1, 24, 48, and 72 hours and 7 days.

Results: Mean Draize score was 4.7 (out of 110) at 1 hour after exposure for the washed eye animals and 0.0 at other points. Nonwashed scores were 3.0 at one hour, 0.3 at 24 hours and 0.0 thereafter.

Remarks: Washing did not reduce irritation.

Reliability: (1) Reliable without restrictions

Reference: Shell Development Company, Westhollow Research Center (1983) Eye Irritation of NEODENE 8 Alpha Olefin in the Rabbit (unpublished report).

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

(2) **Test Substance**

Identity (purity): CAS No. 68526-54-5; Alkenes, C7-9, C8 rich

Method

Method/guideline: Not specified
Type (*test type*): Ocular irritation
GLP: Pre-GLP
Year: 1975
Species/Strain: Albino rabbits
Sex: Males and females
No. of animals per dose: 6
Vehicle: None
Route of administration: Ocular

Test Conditions: The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the right eye of each animal. The upper and lower lids were gently held together briefly to insure adequate distribution of the test material. The contralateral eye in each rabbit served as the control. Throughout the study, food and water were available at all times and animals were housed individually. The age and weight of the test animals were not reported. Statistics used to evaluate the data were not reported.

The general health of each rabbit was examined for irritation of the cornea, iris and conjunctiva at 1 and 4 hours and on days 1, 2, 3, 4 and 7. Ocular reactions were graded according to the Draize Standard Eye Irritation Grading Scale.

Results: Maximum total Draize score = 4

Remarks: There were no animal deaths prior to study termination. The test material produced mild conjunctival irritation which completely cleared within 24 hours

Reliability: (1) Reliable without restrictions

References: Industrial Bio-Test Laboratories, Inc. (1975) Eye Irritation Test - Albino Rabbits (unpublished report).

(3) **Test Substance:** SHOP C68 Internal Olefin

Remarks: CAS No. 25377-72-4, (Pentene=1.9%); CAS No. 25264-93-1, (Hexene=43.3%), CAS No. 25339-56-4, (Heptene=21.7%) and 25377-83-7 (Octene=31.7%), and CAS No. 27215-95-8 (Nonene=1.4%)

Method: OECD Section 405 and Section B5 of Directive 92/69/EEC

Test Type: in vivo

GLP: Yes

Year: 1995

Test Conditions

Species: Rabbits

Strain: New Zealand White

Cell type:

Sex: Female

Number of animals

per dose: 3

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: At the start of the study, the four month old animals supplied by Froxfield SPF Rabbits, Hampshire, England, weighed 2.80 to 3.35 kg. Animals had free access to a commercially available standard pelleted rabbit diet and tap water taken from the public supply. During the acclimatization period, the health status of each animal was monitored and a record kept. Each animal was subjected to a single ocular instillation of 0.1 ml of the test material. Ocular reactions were assessed 1, 24, 48, and 72 hours after treatment.

Results: Very slight or slight conjunctivitis was observed in all animals one hour after instillation, persisting in one animal to the 48 hour examination. The treated eye of each animal was overtly normal by the 72 hour examination. At hour 1, one animal had a score of 2 for redness, two had scores of 1. At 24 hours, 1 rabbit had scores of 1 for redness, 2 animals had scores of 0. At 48 hours, 1 animal had scores of 1 for redness, all other scores were 0. At 72 hours, all scores were 0.

Reliability: (1) Reliable without restrictions

Reference: Huntington Life Sciences Ltd, (1996) SHOP C68 Internal Olefins: Eye Irritation in the Rabbit; Performed for Shell Chemical Co. (unpublished report).

5.4 Skin Sensitisation

A. Test Substance: CAS No. 111-66-0, 1-Octene (1% w/v NEODENE 8 alpha olefin in absolute ethanol)

Method: Buehler
Test Type: challenge
GLP: Yes
Year: 1983

Test Conditions

Species: Guinea pig
Strain: Duncan-Hartley albino
Sex: Males and females

Number of animals per sex per dose: 5

Route of administration: Topical , occluded patch
Induction conc.: 1%
Induction vehicle: Absolute ethanol
Challenge conc.: 1%
Challenge vehicle: Absolute ethanol
Grading system used: 0 = no reaction
+/- = minimal erythema
1 = slight erythema
2 = moderate erythema
3 = moderate erythema with slight edema
4= severe erythema with moderate edema and cracking of skin

Method remarks: DNCB (0.1% w/v) was used as a positive control. Test article and controls were administered 1 day/week, 6 hr/day for 3 weeks. 48 hours prior to dose application, animals were clipped on the back/trunk region using animal clippers. 18-24 hours prior to dosing, the animals were depilated with NEET lotion and rinsed with water. The dose was applied to a 1 inch by 1 inch gauze pad, to the anterior central portion of the clipped area, and secured with BLENDERM surgical tape. The animal was placed in a stainless steel wire restrainer for 6 hours before unwrapping and removal of any excess test materials. The challenge application was accomplished in the same manner, except that, at that time, one patch was placed on the original site and one patch placed on a virgin site immediately posterior to the original patch. The treatment period was the same. The irritation control group was treated only once, on the fifth week and only one patch was applied to these animals.

Results: Negative for sensitization

Grades:

Results Remarks: No increase in irritation over the 5 week test period. At challenge, one test animal compared to 2 vehicle control animals had scores of +/- to 0 at 48 hours.

Reliability: (2) Reliable with restrictions: In the positive control group, 24 hours before the week 2 application, the original site resembled a large open sore. Since the animals were to be treated again, it was decided that they would be treated on the challenge site and that the patch would be covered with BLENDERM tape instead of aluminum foil. The challenge doses were given in the same manner as the sensitizing doses, only they were challenged by placing treatment patch on the right side.

Reference: Shell Development Company, Westhollow Research Center (1983) Guinea Pig Skin Sensitization of NEODENE 8 Alpha Olefin (unpublished report).

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

B. Test Substance: SHOP C68 Internal Olefin

Remarks: CAS No. 25377-72-4, (Pentene=1.9%); CAS No. 25264-93-1, (Hexene=43.3%), CAS No. 25339-56-4, (Heptene=21.7%) and 25377-83-7 (Octene=31.7%), and CAS No. 27215-95-8 (Nonene=1.4%)

Method: OECD Guidelines, Section 406 and Section B6 of Directive 92/69/EEC

Test Type: Magnusson and Kligman

GLP: Yes

Year: 1995

Test Conditions

Species: Albino Guinea pig

Strain: Dunkin-Hartley

Sex: Males and females

Number of animals per sex: 10 each in test group; 5 each in control group

Route of administration: Topical

Intradermal Induction conc.: 50%

Intradermal Induction vehicle: Paraffin oil

Topical
Induction conc.: 100%
Topical
Induction vehicle: none

Challenge conc.: 100% and 30%
Challenge vehicle: Paraffin oil
Positive control: none
Grading system used: Draize

Method remarks: The dorsal trunk and flanks of the 6-8 week old animals, weighing 302-380 grams were clipped on the day prior to dosing. Four males and four females were dosed at 0.4 ml/site at concentrations of 2.5%, 5%, 10%, 25%, and 50% under occlusion with test material for a period of six hours and examined and graded in accordance with the Draize method at 24 and 48 hours after completion of exposure.

A Test Group of 10 male and 10 female animals was dosed topically at 0.4 ml/site under occlusion with test material once per week for three weeks, a total of three induction exposures. A Positive Control Group of 6 males and 6 females was dosed with dinitrochlorobenzene (DNCB). 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 (100% and 0.1% in acetone, respectively) were selected based on the irritation rangefinding phase.

Two weeks after the last induction exposure, Test Group animals were challenge dosed by topical application of a known essentially nonirritating concentration of the test material to previously unexposed areas of skin for six hours. The Positive Control Group was induced and challenged on a similar regimen as the Test Group with DNCB. Reactions to challenge dosing were evaluated at approximately 24 and 48 hours after completion of each exposure.

Results: Negative for sensitization

Grades: See remarks

Results Remarks: Intradermal injection of 50% v/v SHOP C68 in paraffin oil gave rise to isolated cases of slight or moderate erythema and pallor; a similar administration of 50% v/v SHOP C68 in the adjuvant resulted in slight or moderate erythema, pallor, discoloration, eschar formation and edema. The entire suprascapular region of five animals was edematous.

Occluded topical induction application of SHOP C68 gave rise to slight erythema and exfoliation.

Challenge application of test material gave rise to a positive response (slight erythema or a more marked reaction) in sixteen test and four control animals. Challenge of test material in paraffin oil caused a positive response in five test and no control animals. Challenge application of paraffin oil alone caused a positive response in one test and no control animals. Re-challenge application of 50% v/v SHOP C68 in paraffin oil caused a positive response in two test and one control animals. Re-challenge application of paraffin oil alone caused a positive response in one test and no control animals.

Although the incidence of significant responses was slightly higher in test than control animals, the difference was not considered to be sufficiently marked to be attributed to contact sensitization. The reactions were considered to reflect primary irritation. It was therefore concluded that, under the conditions of this study, repeated administration of SHOP C68 did not cause delayed contact hypersensitivity in guinea pigs.

Reliability: (1) Reliable without restrictions

Reference: Huntingdon Life Sciences Ltd. (1996) SHOP Internal Olefin: Delayed hypersensitivity study in the Guinea Pig (Magnusson Kligman Method), Performed for Shell Chemical Co. (unpublished report).

5.5 Repeated Dose Toxicity

Test Substance

Identity (purity): CAS No. 111-66-0, 1-Octene (Netherlands)

Method

Method/guideline: Not specified
Test type: Subchronic (90 day) Gavage
GLP: No
Year: 1986
Species: Rat
Strain: Unknown
Route of Administration: Oral gavage

Duration of test: 90 days
Doses: 0, 5, 50, or 500 mg/kg b.w./day
Sex: Males and females
Exposure period: 7 days/week for 13 weeks
Frequency of treatment: Once daily

Control group and treatment: Concurrent control

Post exposure observation period: None

Statistical methods: Unknown

Test Conditions: Groups of 40 (20M, 20F) rats were gavaged with 0, 5, 50 or 500 mg/kg body weight/day for 7 days a week for 13 weeks. No other details are available.

Results

NOAEL (NOEL): No-toxic-effect level is between 50 and 500 mg/kg b.w./day, and probably only slightly less than 500 mg/kg/b.w./day. Based on data presented, the only NOEL that was determined is 50 mg/kg/day. This is due to the limitations of doses utilized in the study design and treatment related effects observed at 500 mg/kg/day.

LOAEL (LOEL): 500 mg/kg/day

Remarks: Body weights, food intake, clinical signs, behavior, and hematological parameters did not differ significantly. Gross necropsy findings were not different. Slight changes differing from control were only seen in the high dose group, and included increased kidney weights and decreased plasma chloride in both sexes, increased urinary volume and unspecified microscopic kidney differences in male rats only, and increased plasma creatinine in females only.

Reliability: (2) Reliable with restrictions. The study report is not available for review, but was reviewed for SIAM 11.

Flag: Key study for SIDS endpoint.

References: Til, H.P., et al. (1986) Sub-chronic (90-day) Oral Toxicity Study with Octene-1 in Rats. Conducted by Civo Institutes TNO, Report No. V 86.408/251091 for DSM, Beek, the Netherlands, Project No. B 85-1091 (unpublished report).

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

5.6 Genetic Toxicity *in vitro*

A. Gene Mutation

(1) Test Substance

Identity (*purity*): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

Method

Method/guideline: EPA OTS 798.5265
Type: in-vitro bacterial reverse mutation – Ames Assay
System of testing: bacterial
GLP: Yes
Year: 1991
Species/Strain: *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538
Metabolic activation: With and without S9 fraction of livers from rats pretreated with Aroclor 1254

Concentrations tested: 10, 32, 100, 320 and 1000 µg/plate (Doses were based on a pre-test for toxicity)

Statistical Methods: The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose.

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. DMSO was the vehicle for controls. Ethanol was the vehicle for the test material. Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO. The positive controls were 2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine. Three plates were prepared for each dose level.

To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 µg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 1000 µg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates.

A repeat assay was performed in order to verify the data produced in the initial assay.

Results

Cytotoxic conc.: 1000 µg/plate
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material did not produce any evidence of mutagenicity. In the initial and repeat assays, neither a positive response nor a dose related increase in revertants was observed for any of the tester strains either in the presence or absence of metabolic activation. All positive and negative controls responded in a manner consistent with data from previous assays. Under conditions of this assay, the test material was not mutagenic for

the *Salmonella* tester strains at doses up to and including 1000 µg/plate.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint.

References: Exxon Biomedical Sciences, Inc. (1991) Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 111-66-0, 1-Octene (NEODENE 8 Alpha Olefin)

Method

Method/guideline: Ames test, with and without metabolic activation from rat liver homogenate fraction, modification by preincubation plate incorporation

Type: In vitro bacterial reverse mutation – Ames Assay

System of testing: bacterial

GLP: Yes

Year: 1983

Species/Strain: *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538

Metabolic activation: With and without S9 fraction of livers from rats pretreated with Aroclor 1254

Concentrations tested: 0.45 to 1.4 x 10⁻⁴ mg/plate (Doses were based on a pre-test for toxicity)

Statistical Methods: None reported

Test Conditions: Absolute ethanol was the vehicle for the test material. DMSO was the vehicle for positive controls. The positive controls were 2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine. Six glass culture tubes were set up for each dose level of test or control chemical, 3 without and 3 with metabolic activation. The tubes contained 0.50 ml phosphate buffer or S-9/cofactor mix, 0.05 ml solvent, test or control chemical, 0.10 ml bacterial suspension. The tubes were covered with PARAFILM and incubated at 37° C for 20 minutes. Soft agar supplemented with histidine and biotin was added to each tube and the contents poured onto Vogel-Bonner agar plates. The plates were placed into PLEXIGLASS boxes and transferred to 37°C bacterial incubators. After a 2-day incubation, the colonies on each plate were counted with a Biotran II automatic colony counter. Spontaneous reversion rate controls and positive controls for each of the 5 strains were run

concurrently with the mutagenicity assay. Sterility checks as well as strain characterization checks, which included verification of nutritional requirements and reaction of the strains to ampicillin and crystal violet, were also run concurrently. A repeat assay was performed in order to verify the data produced in the initial assay.

Results

Cytotoxic conc.: 0.45 mg/plate
Genotoxic effects: Negative with and without metabolic activation

Remarks: The concentration of the test compound resulting in precipitation: 14 ug/plate to 0.45 mg/plate. No indication of mutagenic response in any of the five *Salmonella typhimurium* strains in presence or absence of metabolic activation fraction.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Shell Development Company, Westhollow Research Center (1983) Assay of NEODENE-8 Alpha Olefin for Gene Mutation in *Salmonella typhimurium* (unpublished report).

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

B. Chromosomal Aberration

(1) Test Substance

Identity (*purity*): CAS No. 111-66-0, 1-Octene (NEODENE 8 alpha olefin)

Method

Method/guideline: Not specified
Type: In-vitro mammalian chromosome aberration test
System of testing: non- bacterial
GLP: Yes
Year: 1983
Cell line: Chinese Hamster Ovary (CHO) cells received from the lab of T.C. Hsu, M.D. Anderson Research Center, Houston, TX

Metabolic activation: With and without S9 fraction. Prepared from the livers of Sprague Dawley rats dosed with Aroclor 1254 at 500 mg/kg body weight.

Concentrations tested: 1 ug to 10 ug/ml

Statistical Methods: The mean and SD of the colony counts from cultures derived from each flask were computed by standard methods.

Test Conditions: Ethanol (95%) was the vehicle for the test material. Positive controls: TEM and CP. Cells were exposed to 6 concentrations of octene in the absence and presence of S-9. The cells were exposed by adding a 0.15 ml aliquot of each concentration of test chemical, positive control chemical or solvent to glass flasks of established cell cultures in log phase growth which contained 15 ml of culture medium either without or with S-9. Negative control cultures were run concurrently. Single cultures were used for the assay. With or without activation, cells for analysis were collected 3, 8, and 12 hrs post exposure, and cells were evaluated using a Coulter ZBI electronic counter. 100 cells from each culture at each time point were scored. A repeat assay was performed in order to verify the data produced in the initial assay.

Results

Cytotoxic conc.: 0.72 mg/ml (Greater than 80% decrease in mean cell number of cells per flask as compared to solvent control, with and without activation).

Genotoxic effects: Equivocal with metabolic activation and negative without metabolic activation.

Remarks: NO ACTIVATION: Aberration rate in mean aberrations per cell and percent abnormal CHO cells from exposure to NEODENE 8 alpha olefin (collected 3, 8, and 12 hours post exposure) not significantly higher than cells exposed to solvent (95% ethanol). Cells collected 12 hours after exposure to culture medium in the absence of S-9 resulted in 0.01 mean aberrations per cell and 1% abnormal cells; those exposed to solvent resulted in 0.06 mean aberrations per cell and 6% abnormal cells. Exposure to TEM resulted in a response of 0.16 mean aberrations per cell and 13% of the cells with aberrations which was significantly higher than that of the solvent control. Cells collected 8 hours after exposure to culture medium in the absence of S-9 resulted in 0.07 mean aberrations per cell and 5% abnormal cells; those exposed to solvent resulted in 0.07 mean aberrations per cell and 7% abnormal cells. Cells collected at 3 hours yielded similar results.

ACTIVATION PRESENT: At 12 hours collection time, cells in the medium control had 0.01 mean aberrations per cell and 1% abnormal cells, while those in the solvent control had 0.04 mean aberrations per cell and 4% abnormal cells. The positive control, CP, produced a response of 0.18 mean aberrations and 14% abnormal cells, significantly higher than that of the solvent control. Exposure to C8 alpha olefin resulted in > 2-fold

increases (compared to solvent control) in aberrations per cell at the 5 highest concentrations, and in percent abnormal cells at 3 nonconsecutive concentrations: 1.8×10^{-3} , 3.2×10^{-3} , and 1×10^{-2} mg/ml. The increases were only slightly over 2-fold the background. Because responses which exceeded 2-fold that of the solvent control were obtained, cells collected at earlier time points under the same conditions were not scored.

Reliability: (2) Reliable with restrictions: Although >15% abnormal cells were not obtained for the positive control, as stated in protocol, the response to TEM and CP were positive (greater than two-fold) when compared to solvent control.

Flag: Key study for SIDS endpoint

References: Shell Development Company, Westhollow Research Center (1983) In Vitro Chromosome Aberration Assay in Chinese Hamster Cells of NEODENE 8 Alpha Olefin (unpublished report).

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

(2) **Test Substance**

Identity (purity): CAS No. 111-66-0, 1-Octene (Netherlands)

Method

Method/guideline: Not specified
Type: In-vitro mammalian chromosome aberration test
System of testing: non- bacterial
GLP: Unknown
Year: 1986
Cell line: Cultured Chinese Hamster Ovary (CHO) cells
Metabolic activation: With and without S9
Concentrations tested: 1.33 to 40 ug/mL
Statistical Methods: Not available

Test Conditions: Cells were exposed for 3 hours to Ham's media, ethanol as solvent control, mitomycin C as positive control without activation or cyclophosphamide as positive control with activation, or to dilutions of test article in ethanol. Harvest times were 12 and 21 hours. No other information is available.

Results

Cytotoxic conc.: 40 ug/mL

Genotoxic effects: Negative with and without metabolic activation.

Reliability: (2) Reliable with restrictions. Report was not available for review.

Flag: Key study for SIDS endpoint

References: Wilmer, J.W.G.M. (1986) Chromosome Analysis of Chinese Hamster Ovary Cells Treated in Vitro with 1-Octene. Conducted by Civo Institutes TNO, Report No. V 86.168/251124, for DSM, Geleen, the Netherlands, Project No. B 85-1124 (unpublished report).

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

C. Other Genetic Effects

Test Substance

Identity (*purity*): CAS No. 111-66-0, 1-Octene (NEODENE 8 Alpha Olefin)

Method

Method/guideline: Not specified
 Type: Morphologic Transformation Assay of BALB/c-3T3
 System of testing: Non-bacterial
 GLP: Yes
 Year: 1983
 Cell line: Mouse embryo cells, BALB/c-3T3
 Metabolic activation: Yes: Adult male Fischer 344 rats dosed with Aroclor 1254 (500 mg/kg body weight) for 5 days prior to sacrifice.

Concentrations tested: Transformation experiment without activation: 62.5 to 16.0 ug/ml
 Transformation experiment with activation: 1.0 to 0.063 mg/ml

Statistical Methods: No data

Test Conditions: Exponentially growing BALB/c-3T3 cells were harvested by trypsinization and were suspended at concentrations of 200-250 cells/ml in growth medium. After adding 2.0-2.5 ml of medium to a 25 cm² flask, 1.0 ml of the cell suspension was added to each of 3 flasks used per concentration of test material and 6 flasks each for the media, acetone and positive control. The dishes were incubated at 37 °C for 18-24 hours.

Dosing in absence of S-9 activation: After the initial incubation period, the medium was removed and replaced with 2.0 ml fresh medium. A solution of each concentration of test chemical was made by diluting a 200x concentration by a factor of 66.7 using growth medium. For dosing, 1.0 ml of this solution was mixed with 2.0 ml of medium. The

cells were then incubated for 3 days at 37⁰ C in the presence of the test chemical.

Dosing in presence of S-9 activation: After the initial incubation period, the medium was removed and replaced with 2.0 ml fresh medium. To a separate tube the following components were added 1) 1.0 ml S-9 liver microsomes adjusted with medium to contain 10x the quantity of protein required for optimal activation of the positive control chemical; 2) 1.0 ml of a solution containing 2.36 mg/ml NADP and 15.52 mg/ml isocitrate adjusted to pH 7.2; 3) 1.0 ml solution made by diluting a 200x concentration of test chemical in ethanol by a factor of 20 with medium; 4) 0.33 ml of medium. The contents of the tube were mixed and added to the 2.0 ml of medium in the dish for 4 hours at 37⁰ C.

The negative controls (15 ul ethanol) and the positive control (MNNG in the absence of S-9 or DMN in the presence of S-9) were used at doses previously found to exhibit activity in the assay.

TOXICITY ASSAY: After 7-8 days, when colonies had developed sufficiently, the growth medium was removed from the flasks, the flasks washed with Hank's Balanced Salt Solution, the cells fixed with 95% methanol for 30 min and stained with Giemsa. The flasks were air dried and the colonies counted by hand.

TRANSFORMATION ASSAY: After exposure to the test chemical for 3 days in the absence of S-9 and 4 hours in the presence of S-9, the cells were washed with Hank's Balanced Salt Solution, refed with growth medium and incubated at 37⁰ C for approximately 4 weeks. Upon termination of the assay, the plates were washed with Hank's Balanced Salt Solution, fixed in 95% methanol, and stained with Giesma.

SCORING OF THE TRANSFORMED FOCI: At the end of the 4-week incubation period, cultures of normal cells yielded a uniformly stained monolayer of round, closely packed cells. Transformed cells formed a dense mass that stained deeply and was superimposed on the surrounding monolayer of normal cells. The foci were variable in size. Foci that had any of these characteristics (random criss-cross orientation, more rounded cells with necrosis at the center or without the necrotic center and large numbers of cells which exhibited criss-cross pattern of overlapping cells throughout the majority of the colony) and exceeded 2 mm in diameter were scored +++, while those less than 2 mm in diameter were designated ++.

Results:

Cytotoxic conc.:

Without activation: ≥ 23.2 ug/ml

With activation: No dose related reductions in cell survival were observed at concentrations of test material as high as 4000 ug/ml. Its transforming activity was tested over the concentration range of 1.0 to 0.063 mg/ml.

Genotoxic effects: Negative

Remarks: No evidence of test material induction of statistically significant increases in transformation frequencies were observed. Test material was considered to be inactive as a BALB/c-3T3 transforming agent in the absence and presence of exogenous metabolic activation.

Reliability: (2) Reliable with restrictions: Test material and positive control chemicals were handled under ambient room light, rather than under yellow light; negative control treatments included the use of culture medium rather than distilled water; MNNG was not used at the positive control in the nonactivated preliminary cytotoxicity test; doses of test material used in the activation study did not include the range of toxicity described in protocol; number of tissue culture vessels used for experimental conditions equaled or exceeded the numbers stipulated in the protocol. In the opinion of the study director, these deviations had no effect on the validity of the data and interpretations.

References: Shell Development Company, Westhollow Research Center (1983) Cell Transformation Assay of NEODENE-8 Alpha Olefin in the Absence and Presence of Microsomal Activation. Performed at Litton Bionetics, Inc., (unpublished report).

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

5.7 Genetic Toxicity *in vivo*

A. Test Substance

Identity (purity): CAS No. 68526-53-4; Alkenes, C6-8, C7 Rich

Method

Method/guideline: EPA OTS 798.5395
Type: Micronucleus Assay
GLP: Yes
Year: 1993
Species: Mouse
Strain: B6C3F1
Sex: Male and female
Route of Administration: Oral gavage
Concentration levels: 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.
Exposure period: Single dose
Statistical methods: Analysis of variance (ANOVA), Duncan's Multiple Range Test. Sexes were analyzed separately.

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. The test material and the carrier (corn oil) were administered by oral gavage as single doses to 15 mice/sex/dose (not fasted). The positive control, cyclophosphamide, was also administered by oral gavage as a single dose of 40 mg/kg. The dosing volume was the same as that of the test material. The test animals were approximately 7 to 9 weeks of age and weighed between 19 and 28 g at the start of the study. Animals from the appropriate groups (5 animals/sex/group) were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended in fetal bovine serum, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. 1000 polychromatic erythrocytes (PCE) from each animal were examined for micronuclei, and the ratio of PCE's to NCE's (normochromatic erythrocytes) was determined for each animal by counting 1000 erythrocytes (PCE's and NCE's).

Results

Effect on PCE/NCE ratio: None
Genotoxic effects: Under the conditions of this study, the test sample is not considered to be mutagenic at doses up to and including 5.0 g/kg.

NOEL: 5.0 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. The test material did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. In addition, the test material did not induce a significant decrease in the mean percent of polychromatic erythrocytes, which is a measure of bone marrow toxicity.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Exxon Chemical Company (1993) In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method (unpublished report).

B. Test Substance

Identity (purity): CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich

Method

Method/guideline: EPA OTS 798.5395
Type: Micronucleus Assay
GLP: Yes
Year: 1991
Species: Mouse
Strain: B6C3F1
Sex: Male and female
Route of Administration: Oral gavage
Concentration levels: 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.
Exposure period: Single dose
Statistical methods: Analysis of variance (ANOVA), Duncan's Multiple Range Test; sexes were analyzed separately

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. The test animals were approximately 8 to 9 weeks of age and weighed between 21 and 29 g at the start of the study. The test material and the carrier (corn oil) were administered by oral gavage as single doses to 15 mice/sex/dose (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose of 40 mg/kg in reagent grade water at the same volume as the test material. Animals from the appropriate groups (5 animals/sex/group) were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended in fetal bovine serum, and prepared for microscopy. Samples were blindly coded and stained with acridine orange. 1000 polychromatic erythrocytes (PCE) from each animal were examined for micronuclei, and the ratio of PCE's to NCE's (normochromatic erythrocytes) was determined for each animal by counting 1000 erythrocytes (PCE's and NCE's)

Results

Effect on PCE/NCE ratio: The test material induced a significant decrease in polychromatic erythrocytes in both males and females at 48 and 72 hours when treated with the high dose (5.0 g/kg). In addition, the mean percent of PCE's for the 5.0 g/kg dose group for both sexes at 48 and 72 hours were statistically different from the carrier controls. The mean percent of PCE's for the female 2.5 g/kg dose group at 48 hours was also statistically different from the carrier control.

Genotoxic effects: Negative.

NOEL: 5.0 g/kg

Remarks: There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. Thus, 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 responded appropriately and is clastogenic. These observations indicate that the test material was toxic to mouse bone marrow at higher concentrations, but did not induce micronuclei formation. Under conditions of this assay, the test material is not considered clastogenic in mice up to and including 5.0 g/kg when evaluated up to 72 hours after dose administration.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Exxon Biomedical Sciences, Inc. (1991) In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method (unpublished report).

5.8 Carcinogenicity

No data available

5.9 Reproductive Toxicity (including Fertility and Developmental Toxicity).

A. Fertility

No data available

B. Developmental Toxicity

No data available

5.10 Other Relevant Information

Aspiration

Test Substance

Identity: C6-C18 even numbered alpha olefins

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 C₈ to C₁₄ died within 24 hours. With C₁₆ and C₁₈, there was only one death (C₁₈). 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 C₆ to C₁₄ 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-octene at SIAM 11.

5.11 Experience with Human Exposure

No data available

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