

201-15896F

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

ROBUST SUMMARIES DOSSIER

for

C7 MEMBERS

of the

HIGHER OLEFINS CATEGORY

Members containing C7 olefins:

CAS No. 25339-56-4, Heptene

CAS No. 68526-53-4, Alkenes, C6-8, C7-Rich

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

* Addressed in the C8 dossier

Contains Robust Summaries for the Following Substances:

CAS No. 25339-56-4, Heptene

CAS No. 592-76-7, 1-Heptene

CAS No. 68526-53-4; Alkenes, C6-8, C7-Rich

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

C6-C8 Internal Olefins

Prepared by:

**American Chemistry Council
Higher Olefins Panel**

April 28, 2005

05 JUN 30 AM 10:00

RECEIVED
OPPT/OMD

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 is sponsoring 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	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9

C12,14 Olefin rich hydrocarbons	Linear	68514-33-0
---------------------------------	--------	------------

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: Heptene is manufactured and marketed as a component of a blend, and Alkenes, C6-8, C7-rich is a blend.

1.2 Impurities

Remark: The compositions reported by manufacturers are shown below:

Heptene	25339-56-4	C6-C8 internal olefin blend: Typical composition = 1.9% C5, 43.3% C6, 21.7% C7, 31.7% C8, 1.4% C9
Alkenes, C6-8, C7 rich	68526-53-4	Typical composition: 1% C6 olefins, 97% C7 olefins, 2% C8 olefins.

1.3 Additives

None

1.4 Synonyms

Some synonyms are: heptene, Isomer(s)
 Heptylene
 Heptenes

1.5 Quantity

Remarks: Range of U.S. production volumes for 2002 submitted by Higher Olefin Panel members to Panel Manager:
 CAS No. 25339-56-4, Heptene = 50-100 million pounds; CAS No. 68526-53-4; Alkenes, C6-8, C7 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, 2000). 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
Length of
Exposure period:
Frequency:

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

E. Other Remarks

2. PHYSICAL CHEMICAL DATA

2.1 Melting Point

A. Test Substance

Identity: CAS No. 25339-56-4, Heptene or CAS No. 68526-53-4; Alkenes, C6-8, C7 rich

Method

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

GLP: Not applicable
Year: Not applicable

Test Conditions: 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-heptene.

Results

Melting point value in °C: -82.42°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 (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: 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)

C. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

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

Test Conditions: No data

Results

Melting point
value in °C: -119.7°C

Reliability: (2) Reliable with restrictions. The result is an experimental value in the EPIWIN database and in a secondary source (Lide, 1998-1999), and data were not reviewed for quality.

Flag: Key study for SIDS endpoint

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

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

2.2 Boiling Point

A. Test Substance

Identity: CAS No. 25339-56-4, Heptene or CAS No. 68526-53-4; Alkenes, C6-8, C7 rich

Method

Method/
guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP: Not applicable
Year: Not applicable

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). The program used the structure for 1-heptene.

Results

Boiling point
value in °C: 94.35°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 (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: 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

C. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

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

Test Conditions: No data

Results

Boiling point value: 93.6°C
pressure: 1013
Pressure unit: hPa

Reliability: (2) Reliable with restrictions. Result is an experimental value in the EPIWIN database and in another secondary source (Lide, 1998-1999). These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

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

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

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 from a reliable source but were not reviewed for quality.

Reference: Shell Chemicals UK Ltd. Chester

2.4 Vapour Pressure

A. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

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

Test Conditions:**Results**

Vapor Pressure
Value: 79.05 hPa
Temperature: 25°C
Remarks: Reported as 59.3 mm Hg (25°C)

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

Flag: Key study for SIDS endpoint

References: Daubert, T.E. and R.P. Danner (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY

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

B. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

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

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. Used experimental value for BP of 93.6 °C from EPIWIN database

Results

Vapor Pressure
value: 74.66 hPa
Temperature (°C): 25°C
Remarks: Reported as 56 mm Hg

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

Flag: Key study for SIDS endpoint

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

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

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

C. Test Substance

Identity: CAS No. 68526-53-4; Alkenes, C6-8, C7 rich

Method

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

GLP: Not applicable

Year: Not applicable

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. Used experimental value for BP of 93.6 °C (for 1-heptene) from EPIWIN database

Results

Vapor Pressure
value: 74.66 hPa
Temperature (°C): 25°C
Remarks: Reported as 56 mm Hg

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

Flag: Key study for SIDS endpoint

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

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

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

2.5 Partition Coefficient (log₁₀K_{ow})

A. Test Substance

Identity: C6-C8 Internal Olefins

Method

Method: No data

GLP: No data

Year: No data

Test Conditions: No data

Results

Log K_{ow}: 3.4 – 4.6

Reliability: (4) Not assignable. Limited information was available and these data were not reviewed for quality.

References: Shell Chemicals UK Ltd. Chester

B. Test Substance

Identity: CAS No. 25339-56-4, Heptene or CAS No. 68526-53-4; Alkenes, C6-8, C7 rich

Method

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

GLP: Not applicable
Year: Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Experimental Log Kow value of 3.99 for 1-heptene from EPIWIN database used for calculation. Program used structure for 1-heptene.

Results

Log Kow: 3.64
Temperature (°C): Not applicable

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

Flag: Key study for SIDS endpoint

Reference: Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.
EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

Method: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Log Kow: 3.99
Temperature (°C): No data

Reliability: (2) Reliable with restrictions. The result is an experimental value in the EPIWIN database and the 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. Washington, DC: American Chemical Society.

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

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

2.6.1 Water Solubility (including *Dissociation Constant).**A. Test Substance**

Identity: CAS No. 25339-56-4, Heptene or CAS No. 68526-53-4; Alkenes, C6-8, C7 rich

Method

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

Test Conditions: Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an experimental Log Kow of 3.99, from the EPIWIN database.

Results

**Value(mg/L) at
temperature (°C):** 13.45 mg/L (25°C)

Reliability: (2) Reliable with restrictions. The result was calculated by EPIWIN using experimental data from the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

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

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

B. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

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

Test Conditions: No data

Results

Value (mg/L)
at temperature (°C): 18.2 mg/L (25°C)

Reliability: (2) Reliable with restrictions. The 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 (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

Method/
guideline followed: Calculated value using the computer program EPIWIN, WATERNT v 1.01
GLP: Not applicable
Year: Not applicable

Test Conditions: The calculation was based on chemical structure as modeled by EPIWIN.

Results

Value(mg/L) at
temperature (°C): 11.913 mg/L (25°C)

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

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

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. Data were from a reliable source but 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

2.13 Additional Information

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 Stability

A. Photodegradation

(1) Test Substance

Identity: CAS No. 25339-56-4, Heptene ; or CAS No. 68526-53-4;
Alkenes, C6-8, C7 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. 25339-56-4, Heptene

Method

**Method/
guideline followed:** Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11. Program used structure for 1-heptene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser (type): OH
Rate Constant: 31.5910 E-12 cm³/molecule-sec
Degradation % after: 50% after 4.063 hrs (using 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: EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(3) Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

Method/
guideline followed: Measured value cited in the experimental database of the
computer program EIPWIN version 3.11

Type: air
GLP: No data
Year: No data

Results

Indirect photolysis

Sensitiser (*type*): OH
Rate Constant: 40.5 E-12 cm³/molecule-sec
Sensitiser (*type*): Ozone
Rate Constant: 1.73 E-17 cm³/molecule-sec

Reliability: (2) Reliable with restrictions. The value is from the
experimental database in EPIWIN and data were not evaluated
for quality.

References: Atkinson, R (1989); EPIWIN (2000). Estimation Program
Interface for Windows, version 3.11. EPI Suite™ software, U.S.
Environmental Protection Agency, Office of Pollution
Prevention and Toxics, U.S.A.

B. Stability in Water

Test Substance

Identity: CAS No. 25339-56-4, Heptene; or CAS No. 68526-53-4; Alkenes, C6-8,
C7 rich

Method

Method/
guideline followed: Other – Technical Discussion

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 C7 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. 25339-56-4, Heptene

Method

Type: Fugacity models, Mackay Levels I and III

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

Chemical assumptions:

Molecular weight: 98
Water solubility: 13.5 g/m³
Vapor pressure: 7466 Pa (25°C)
Log Kow: 3.99
Melting point: -82.42°C
Environment name: EQC Standard Environment

Half-life in air = 4.5 hr, half-life in water = 208 hr, half-life in soil = 208 hr, half-life in sediment = 832 hr

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

Results

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

	Level I	Level III
Air	100%	7.7%
Water	<1%	79.5%
Soil	<1%	11%
Sediment	<1%	1.6%

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

Conclusions: These results indicated that heptene 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: Input data are calculated.

Flag: Critical study for SIDS endpoint

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

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

B. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

Type: Volatilization from water

Remarks: Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 0.421 atm·m³/mole (HENRY experimental database) and EPIWIN default values

Results: Half-life from a model river: 1.013 hrs
Half-life from a model lake: 3.9 days

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

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

3.3.2 Distribution

A. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

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

Test Conditions: Based on chemical structure; program used chemical structure for 1-heptene

Results

Value: Estimated Koc = 275

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

B. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

Method: Henry's Law Constant calculated value using the computer program EPIWIN, HENRY 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 = 56 mm Hg and WS = 13.4 mg/L. (program used structure for 1-heptene)

Results

Value: Bond estimate = 0.476 atm-m³/mole
Group estimate = 0.756 atm-m³/mole
VP/Wsol estimate = 0.5379 atm-m³/mole

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

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

C. Test Substance

Identity: CAS No. 592-76-7, 1-Heptene

Method

Method: Henry's Law Constant – experimental data from EPIWIN v. 3.11 database

Test Conditions: No data

Results

Value: 0.421 atm-m³/mole

Reliability: (2) Reliable with restrictions. Result is from the EPIWIN experimental database and data were not reviewed for quality.

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

3.4 Aerobic Biodegradation**A. Test Substance**

Identity: CAS No. 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) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119194A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

B. Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

Method/guideline: Estimated using the computer program EPIWIN v 3.10, BIOWIN v 4.01
Type: Aerobic

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

Results: Linear model prediction: Biodegrades fast
Non-linear model prediction: Biodegrades fast
Ultimate biodegradation timeframe: Days-Weeks
Primary biodegradation timeframe: Days
MITI linear model prediction: Biodegrades fast

MITI non-linear model prediction: Biodegrades fast

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

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

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

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

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

3.5 BOD5, COD or ratio BOD5/COD

No data available

3.6 Bioaccumulation

Test Substance

Identity: CAS No. 25339-56-4, Heptene

Method

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

Test Conditions: Based on chemical structure and Log Kow of 3.99 (EPIWIN experimental database). Formula used to make BCF estimate: $\text{Log BCF} = 0.77 \log \text{Kow} - 0.70$ with no correction factor.

Results

Value: Estimated Log BCF = 2.372 (BCF = 235.7)

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

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

3.7 Additional Information

Sewage Treatment

Test Substance

Identity: CAS No. 25339-56-4, Heptene

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.
Input values: MW = 98.19; Henry's LC = 0.421 atm-m³/mol; air-water partition coefficient = 17.2176; Log Kow = 3.99; biomass to water partition coefficient = 1955.27; temperature = 25°C

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results: 99.47 % removed from wastewater treatment

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

4. ENVIRONMENTAL TOXICITY

4.1 Acute Toxicity to Fish

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 22°C).

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) Fish Acute Toxicity Test. Study #119158. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

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

No data available

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

No data available

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

No data available

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

Test Substance: CAS No. 25339-56-4, Heptene; or CAS No. 68526-53-4; Alkenes, C6-8, C7 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, 2000)

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 3.64 for both substances. The Kow value was estimated by EPIWIN using the structure for 1-heptene.

Results:

Units/Value: Estimated 30-day ChV = 351 µg/L for both substances

Flag: Key study for SIDS endpoint

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

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

B. Chronic Toxicity to Aquatic Invertebrates

Test Substance: CAS No. 25339-56-4, Heptene; CAS No. 68526-53-4; Alkenes, C6-8, C7 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, 2000)

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 3.64 for both substances. The Kow value was estimated by EPIWIN using the structure for 1-heptene.

Results:

Units/Value: Estimated 16-day EC50 = 264 µg/L for both substances

Flag: Key study for SIDS endpoint

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

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

4.6 Toxicity to Terrestrial Organisms

A. Toxicity to Terrestrial Plants.

Test Substance: CAS No. 25339-56-4, Heptene ; CAS No. 68526-53-4; Alkenes, C6-8, C7 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, 2000)

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 3.64 for both substances. The Kow value was estimated by EPIWIN using the structure for 1-heptene.

Results:

Units/Value: Estimated 96-hr ChV = 445 µg/L for both substances

Flag: Key study for SIDS endpoint

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

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

B. Toxicity to Soil Dwelling Organisms.

No data available

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

No data available

4.7 Biological Effects Monitoring (including Biomagnification)

No data available

4.8 Biotransformation and Kinetics

No data available

5. MAMMALIAN TOXICITY

5.1 Toxicokinetics, Metabolism and Distribution

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 µmoles 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 µmoles 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 µmoles 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 µmoles n-1-octene contained both 1,2-epoxy-n-octane (0.40 µmoles) and n-octane-1,2-diol (0.23 µmoles), whereas in the absence of the inhibitor, only the glycol (0.64 µmoles) 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. 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, <i>cis</i> and <i>trans</i> 2-nonene, 4-ethyl-1-hexene, and 3-methyl-1-octene at a dose of 400 µl/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:	<i>In vitro</i> : Hepatic microsomal cytochrome P-450 was destroyed <i>in vitro</i> , in the presence of NADPH, by 4-ethyl-1-hexene, 3-methyl-1-octene, and 1-heptene. The <i>cis</i> - and <i>trans</i> -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-nonenenes 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.

C. 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

D. Test Substance: CAS No. 592-76-7, 1-Heptene

Method
Test Type: In vivo

GLP
Year

No data available
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-heptene] 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 $\mu\text{mol/kg}$; 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-hexene, will be genotoxic or carcinogenic under these conditions.

- Reliability:** (1) Reliable without restrictions.
- Reference:** Eide, I., R. Hagerman, K. Zahlse, 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. Additional information has been added.

5.2 Acute Toxicity

A. Acute oral toxicity

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 with Alkenes, C7-9, C8 Rich (unpublished report).

B. Acute inhalation toxicity

Test Substance

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

Method

Method/guideline: NA
Type (*test type*): LC50
GLP: Pre-GLP
Year: 1979
Species/Strain: Swiss albino Mice, Sprague-Dawley Rats, Hartley Guinea Pigs
Sex: Males and Females
No. of animals
per sex per dose: 5

Vehicle: None
Route of
administration: Inhalation - vapor

Test Conditions: Age of the test animals was not reported. Body weights ranged from 17 to 23 g (mice), 187 to 260 g (rats), and 293 to 381g (guinea pigs) at initiation of the study. Animals were given a single dose of test substance vapor at a concentration of 42.3 mg/L (10,533 ppm) for 6 h.

Control animals (5/sex/species) were exposed to clean air as a sham exposure.

Room air, at a flow rate of 134 l/minute was bubbled through test material in a flask to produce a vapor-laden airstream that was directed, undiluted, into the exposure chamber. The nominal exposure concentration was calculated by dividing the mass of test material consumed by the total volume of air passing through the chamber. For the purpose of this study, the test material was considered to be free of impurities.

Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. During the necropsies, the lungs with trachea, kidneys, and liver were preserved for possible histopathological examination. The statistics used to analyze the data were not reported.

Results

Value: LC50 > 42.3 mg/L (10,533 ppm) for 6 h

Number of deaths at each dose level:

One female mouse died 1 hr into the exposure period. Two guinea pigs (1 male and 1 female) died by 45 minutes into the exposure period. No rats died during the study.

Remarks:

In mice, exposure to 42.3 mg/L of the test substance resulted in 1 death (female) 1 hour into the exposure period. All other mice survived until the end of the study. None of the rats died during the study. Two guinea pigs (1 male and 1 female) died by 45 minutes into the exposure period. The remaining guinea pigs survived until the end of the study. All exposed species exhibited signs of systemic toxicity including labored breathing, prostration, body tremors, and ataxia during the exposure. However, in the surviving animals, these signs completely reversed within 24 hours following the exposure. Liver discoloration was noted upon necropsy in the mouse and the two guinea pigs that died during the exposure. Otherwise, no significant findings were observed at necropsy. Under conditions of this study, Alkenes, C6-8, C7 rich have a low order of acute inhalation toxicity in rodents.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Bio/dynamics, Inc. (1979) An Acute Inhalation Toxicity Study of MRD-ECH-78-32 in the Mouse, Rat, and Guinea Pig. Conducted for Exxon Research and Engineering Company (unpublished report).

C. Acute dermal toxicity

Test Substance

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

Method

Method/guideline: Not specified
Type (*test type*): LD50
GLP: Pre-GLP
Year: 1978
Species/Strain: New Zealand White rabbits
Sex: Males and females
No. of animals per sex per dose: 2
Vehicle: None
Route of administration: Dermal

Test Conditions: For the purpose of this study, the test material was considered to be free of impurities. Concentration levels were 200 and 3160 mg/kg. Test animals were at least 9 weeks old and weighed between 2.2 and 3.3 kg at the start of the study. Undiluted test material was applied to clipped, abraded abdominal skin under gauze and thick plastic. Following the 24-hour exposure period, the wrapping was removed and the exposed area was wiped to remove residue. Animals were observed for gross signs of irritation and systemic toxicity 1,2,3, and 4 hours post dose and daily for 14 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. 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: Lethargy and ataxia were observed in all animals, but these symptoms cleared by Day 2. Dermal reactions were generally moderate at 200 mg/kg and cleared by Day 14. In the high dose group, more severe dermal reactions, including moderate edema and severe erythema, persisted through the study. No significant fluctuations in body weight occurred. Necropsy findings were unremarkable except for a pus-filled liver in 1 rabbit from the high dose group. Under the conditions of this study, Alkenes, C6-8, C7 rich have a low order of acute dermal toxicity.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: MB Research Laboratories, Inc. (1978) Acute Dermal Toxicity in Albino Rabbits (unpublished report).

D. Acute toxicity, other routes

No data available

5.3 Corrosiveness/Irritation

A. Skin Irritation/Corrosion

Test Substance

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

Method

Method/guideline: Not specified

Type (*test type*): Dermal irritation

GLP: Pre-GLP

Year: 1978

Species/Strain: Albino rabbits

Sex: Males and females

**No. of animals
per sex per dose:** 2

Vehicle: None

**Route of
administration:** Dermal

Test Conditions: Concentration levels were 200 and 3160 mg/kg. Undiluted test material was applied to clipped, abraded abdominal skin under gauze and thick plastic. Following the 24-hour exposure period, the wrapping was removed and the exposed area was wiped to remove residue. Animals were observed for gross signs of irritation and systemic toxicity 1,2,3, and 4 hours post dose and daily for 14 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. Test animals were at least 9 weeks old and weighed between 2.2 and 3.3kg at the start of the study. Statistics used to evaluate the data were not reported.

Results:

Value: Irritant

Dermal Scores

<u>Dose Level</u>	<u>Erythema</u>		<u>Edema</u>	
	<u>Mean</u>	<u>Max</u>	<u>Mean</u>	<u>Max</u>
200 mg/kg	1.4	2.0	0.5	1.5
3160 mg/kg	2.6	3.0	1.3	2.3

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

Remarks: Dermal reactions were generally moderate at 200 mg/kg and cleared by Day 14. In the high dose group, more severe dermal reactions, including moderate edema and severe erythema, persisted through the study. No significant fluctuations in body weight occurred. Necropsy findings were unremarkable except for a pus-filled liver in 1 rabbit from the high dose group.

Reliability: (1) Reliable without restrictions

References: MB Research Laboratories, Inc. (1978) Acute Dermal Toxicity in Albino Rabbits (unpublished report).

B. Eye Irritation/Corrosion

(1) Test Substance

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

Method

Method/guideline: Not specified
Type (*test type*): Ocular irritation
GLP: Pre-GLP
Year: 1978
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. Test animals were at least

9 weeks old and weighed between 1.8 and 3.5kg at the start of the study. 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 = 15

Remarks: There were no animal deaths prior to study termination. Based on these findings, this test material is neither an irritant or a non-irritant according to the criteria of this test. Slight to moderate irritation was noted at the first and fourth hour. Slight irritation continued to Day 2 in two rabbits.

Reliability: (1) Reliable without restrictions

References: MB Research Laboratories, Inc. (1978) Eye Irritation in Albino Rabbits (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 68526-53-4; Alkenes, C6-8, C7 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 was 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 = 15

Remarks: There were no animal deaths prior to study termination. All observations were completely cleared by 72 hours. Based on these findings, this test material was minimally irritating. Slight to moderate irritation was noted at the first and fourth hour.

Reliability: (1) Reliable without restrictions

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

5.4 Skin Sensitisation

No data available

5.5 Repeated Dose Toxicity

No data available

5.6 Genetic Toxicity *in vitro*

A. Gene Mutation
No data available

B. Chromosomal Aberration
No data available

5.7 Genetic Toxicity *in vivo*

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).

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: C6-18 even carbon 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.

5.11 Experience with Human Exposure

No data available

6.0 References

American Chemistry Council's Higher Olefins Panel (2002) Personal communication.

Atkinson, R (1989); EPIWIN (2000). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

Bio/dynamics, Inc. (1979) An Acute Inhalation Toxicity Study of MRD-ECH-78-32 in the Mouse, Rat, and Guinea Pig. Conducted for Exxon Research and Engineering Company (unpublished report).

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.

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

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.

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

Exxon Biomedical Sciences, Inc. (1996) Fish Acute Toxicity Test. Study #119158. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119194A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

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

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 with Alkenes, C7-9, C8 Rich (unpublished report).

Gerarde, H.W. (1963) Toxicological Studies on Hydrocarbons. *Archives of Environmental Health* 6:329-341.

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

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

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

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.

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.

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

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.

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

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.

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.

MB Research Laboratories, Inc. (1978) Acute Dermal Toxicity in Albino Rabbits (unpublished report).

MB Research Laboratories, Inc. (1978) Eye Irritation in Albino Rabbits (unpublished report).

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

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.

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

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

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.

NLM (2003). TRI (Toxic Release Inventory). U.S. National Library of Medicine, Specialized Information Services, National Institutes of Health, Department of Health and Human Services. September 2003 (<http://toxnet.nlm.nih.gov>).

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.

Shell Chemical Company MSDS

Shell Chemicals UK Ltd. Chester

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

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>)

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)

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

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

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