

201-15896N

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

ROBUST SUMMARIES DOSSIER

for

C10 MEMBERS

of the

HIGHER OLEFINS CATEGORY

Members containing C10 olefins:

CAS No. 68855-58-3 Alkenes, C10-16 alpha
CAS No. 68526-55-6; Alkenes, C8-10, C9-Rich
CAS No. 68526-56-7; Alkenes, C9-11, C10-Rich
CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich
CAS No. 68991-52-6; Alkenes, C10-16
CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Contains Robust Summaries for the Following Substances:

CAS No. 25339-53-1, Decene
CAS No. 872-05-9, 1-Decene
CAS No. 68526-56-7; Alkenes, C9-11, C10-Rich
CAS No. 85535-87-1, Alkenes C10-13
C10-13 Internal olefins (SHOP Olefins 103PQ11/Olefins 103 PQ11/SHOP Olefins 103)
CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Prepared by:

**American Chemistry Council
Higher Olefins Panel**

April 28, 2005

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

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

A. Type of Substance

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

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

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

C. Purity: C10 containing category members are manufactured and marketed as blends

1.2 Impurities

Remark: The compositions reported by manufacturers for the members of the Higher Olefins Category containing C10 olefins are shown below:

Alkenes, C10-16 alpha	68855-58-3	Typical composition: 0.6% C10, 64.2% C12, 34.7% C14, 0.5% C16; 99.6% monoolefin; 0.4% paraffin; 86.5% linear terminal; 10.6% branched terminal; 2.9% linear internal
Alkenes, C8-10, C9-rich	68526-55-6	Mostly linear, less than 2% branched. Typical composition: 1% C8 olefins, 91% C9 olefins, 8% C10 olefins.
Alkenes, C9-11, C10-rich	68526-56-7	Mostly linear, less than 2% branched. Typical composition: 5% C9 olefins, 84% C10 olefins, 10% C11 olefins, 0.2% C12 olefins; or Max. 5% C9 and lower, minimum 94% C10, max. 3% C11 and higher, max. 10% branched
Alkenes, C10-12, C11-rich	68526-57-8	Typical composition: 1% C9 olefins, 10% C10 olefins, 76% C11 olefins, 13% C12 olefins. Also reported: Mostly linear, less than 2% branched
Alkenes, C10-16	68991-52-6	Mostly linear, less than 2% branched.
C10,12 Olefin rich hydrocarbons	68514-32-9	0-1% C8, 10-30% C10, 70-90% C12, 0-1% C14, 0-50% paraffins

1.3 Additives

None

1.4 Synonyms

1.5 Quantity

Remarks: Range of U.S. production volumes for 2002 submitted by Higher Olefin Panel members to Panel Manager:
CAS No. 68855-58-3 Alkenes, C10-16 alpha = 1-10 million pounds
CAS No. 68526-55-6; Alkenes, C8-10, C9 Rich = 300-400 million pounds
CAS No. 68526-56-7; Alkenes, C9-11, C10-rich = 50-100 million pounds
CAS No. 68526-57-8; Alkenes, C10-12, C11-rich = 50-100 million pounds
CAS No. 68991-52-6; Alkenes, C10-16 = 400-500 million pounds
CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons = 1-10 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
Intermediate

Remarks:

Intermediate in the manufacture of plasticizer and detergent alcohols, surfactants, nonionics, polyalphaolefins and other additives for lubricants, amine oxides and amines

(b) Main
Industrial
Use

Non-dispersive use
Chemical industry – chemicals used in synthesis
Intermediate

Remarks:

Intermediate in the manufacture of plasticizer and detergent alcohols, surfactants, nonionics, polyalphaolefins and other additives for lubricants, amine oxides and amines

B. Uses In Consumer Products

Not applicable

1.7 Sources of Exposure

Remarks: These products are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals. 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: Biotreater, burned for fuel

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. 872-05-9, 1-Decene

Method No data
GLP: No data
Year: No data

Results:
Melting point
Value: -66.3 °C

Decomposition: No data
Sublimation: No data

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

Flag: Key study for SIDS endpoint

References: 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. 25339-53-1, Decene

Method: ASTM D97
GLP: Yes [] No[X]
Year: 1978
Remarks: value is for pour point

Results:
Melting point
Value: -66 °C:

Decomposition: Yes [] (*temperature* °C) No [X] Ambiguous []
Sublimation: Yes [] No [X] Ambiguous []

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

References: Enichem Augusta Ind. Technical Bulletin

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

C. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method/

guideline followed: Calculated value using MPBPWIN version 1.40, a subroutine of 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. Program used the structure for 1-decene

Results

Melting point value in °C: -45.48°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 (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

D. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 Rich

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

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin. Program used a C10 structure with double bonds in 3 locations.

Results

Melting point value in °C: -46.73°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.

E. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

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

GLP: Not applicable

Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin. Program used a C10 structure with double bonds in 5 locations.

Results

Melting point value in °C: -48.73°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. 872-05-9, 1-Decene

Method

Method: No data

GLP: No data

Year: No data

Results

Boiling point value: 170.5°C

Pressure: 1013

Pressure unit: hPa

Decomposition: No data

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

Flag: Key study for SIDS endpoint.

References: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection

B. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

Method: No data

GLP: No data

Year: No data

Results

Boiling point value: 170°C

Pressure: 1013

Pressure unit: hPa

Decomposition: No data

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

Flag: Key study for SIDS endpoint.

References: 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.

C. Test Substance

Identity: CAS No. 25339-53-1, Decene

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). Program used the structure for 1-decene.

Results

**Boiling point
value in °C:** 162.99°C

Pressure: 1013

Pressure unit: hPa

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

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

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

D. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 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). Program used a C10 structure with double bonds in 3 locations.

Results

Boiling point value in °C: 176.08°C
Pressure: 1013
Pressure unit: hPa

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

Flag: Key study for SIDS endpoint

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

E. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

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

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used a C10 structure with double bonds in 5 locations.

Results

Boiling point value in °C: 181°C
Pressure: 1013
Pressure unit: hPa

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

Flag: Key study for SIDS endpoint

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

2.3 Density (Relative Density)

A. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

Method: ISO 3675
GLP: Yes No ?

Results

Type:
Value: 740 kg/m³
Temperature: (20°C)

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

Reference: Shell Chemicals UK Ltd, Chester as cited in IUCLID

B. Test Substance

Identity: 4-Decene, 5-Decene

Method

Method: No data
GLP: No data

Results

Type:
Value: 0.74 g/cm³
Temperature: (20°C)

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

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

2.4 Vapour Pressure

A. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

Method: No data
GLP: Yes [X] No []

Results

Vapour Pressure value: 1.33 hPa
Temperature: 14.7°C
Decomposition: Yes [] No [x] Ambiguous []

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

References: Verschueren, K. (1983) *Handbook of environmental data on organic chemicals*, 2nd ed. Van Nostrand Reinhold, NY. P 448.

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

B. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

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

Test Conditions: No data

Results

**Vapor Pressure
Value:** 2.23 hPa
Temperature: 25°C
Remarks: Reported as 1.67 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 (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

**Method/
guideline followed:** Calculated value using the computer program EPIWIN v. 3.10, MPBPWIN v 1.40

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. The calculation used an experimental value for BP of 170 °C from EPIWIN database. Program used the structure for 1-decene.

Results

**Vapor Pressure
value:** 2.79 hPa
Temperature (°C): 25°C
Remarks: Reported as 2.09 mm Hg

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

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.

D. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 Rich

Method

**Method/
guideline followed:** Calculated value using the computer program EPIWIN v. 3.11, 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. The calculation used a value for BP of 176.08 °C estimated by EPIWIN which was estimated using a C10 structure with double bonds in 3 locations.

Results

**Vapor Pressure
value:** 2.11 hPa
Temperature (°C): 25°C
Remarks: Reported as 1.58 mm Hg

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

Flag: Key study for SIDS endpoint

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

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

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

E. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

**Method/
guideline followed:** Calculated value using the computer program EPIWIN v. 3.11,
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. The calculation used a value for BP of 181°C estimated by EPIWIN which was estimated using a C10 structure with double bonds in 5 locations.

Results

Vapor Pressure
value: 1.6932hPa
Temperature (°C): 25°C
Remarks: Reported as 1.27 mm Hg

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

Flag: Key study for SIDS endpoint

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

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

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

2.5 Partition Coefficient (log10Kow)

A. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

GLP: No data
Year: 1979

Results

Log Kow: 5.4
Temperature: 20 °C
Remarks: Material is not miscible with water

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

References: Hansch C. and A. Leo (1979) *Substituent constants for correlation analysis in chemistry and biology*, Wiley, New York.

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

B. Test Substance

Identity: CAS No. 25339-53-1, Decene

Method

Method: Calculated value using the computer program EPIWIN version 3.10, 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). Program used the structure for 1-decene.

Results

Log Kow: 5.12
Temperature (°C): Not applicable

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

Flag: Key study for SIDS endpoint

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

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

C. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

GLP: No data

Year: No data

Results

Log Kow: 5.7

Temperature:

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

Flag: Key study for SIDS endpoint

References: American Petroleum Institute (1994) as cited in 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.

D. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 Rich

Method

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

GLP: Not applicable

Year: Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used a C10 structure with double bonds in three locations.

Results

Log Kow: 4.69

Temperature (°C): Not applicable

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

Flag: Key study for SIDS endpoint

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

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

E. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

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

GLP: Not applicable

Year: Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used a C10 structure with double bonds in 5 locations.

Results

Log Kow: 4.33

Temperature (°C): Not applicable

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

Flag: Key study for SIDS endpoint

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

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

2.6.1 Water Solubility (including *Dissociation Constant).

A. Test Substance

Identity: CAS No. 25339-53-1, Decene

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 5.70 (for 1-decene).

Results

Value(mg/L) at
temperature (°C): 0.3288 mg/L (25°C)

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

Flag: Key study for SIDS endpoint

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

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

B. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

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

Test Conditions: No data

Results

Value (mg/L)

at temperature (°C): 0.57 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: Kertes, A.S. (1989) Selective transport of hydrocarbons in the unsaturated zone due to aqueous and vapor phase partitioning . Water Resources Research 23, 1926-38; EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

**Method/
guideline followed:** Not reported

GLP: No

Year: 2004

Test Conditions: An equilibrium study was performed to measure the solubility of 1-decene in the test medium for a *Daphnia magna* Reproduction Test conducted in accord with OECD 211 Test Guideline under identical conditions used to generate the stock exposure solution for the in-life phase of the reproduction study. A "gas saturation" method was employed to determine the feasibility and duration required for the test substance to achieve an equilibrium concentration using the following procedure: The test substance was aerated and the vapor passed into an aspirator bottle containing vehicle/dilution medium. 1-Decene saturated vapor passed through an air stone near the bottom of the aspirator bottle providing maximum contact between the test substance in the vapor phase and vehicle/dilution medium. The method of analysis was automated static headspace gas chromatography with flame ionization detection (HS GC-FID). Samples were analyzed using a Perkin-Elmer HS 40 Headspace Sampler connected to a Perkin Elmer AutoSystem XL Gas Chromatograph with flame ionization detection. Analytical standards were prepared and analyzed at concentrations bracketing the sample concentrations.

Results

**Value (mg/L)
at temperature (°C):** 0.210 mg/L (25°C)

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

References: ExxonMobil Biomedical Sciences, Inc. (2004). *Daphnia magna* Reproduction Test with 1-DECENE. Study # 180446. Performed at ExxonMobil Biomedical Sciences, Inc. Annandale, NJ, for the American Chemistry Council.

D. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 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 estimated Log Kow of 4.69 (estimated using a C10 structure with double bonds in 3 locations).

Results

**Value(mg/L) at
temperature (°C):** 2.51 mg/L (25°C)

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

Flag: Key study for SIDS endpoint

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

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

E. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

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

Year: Not applicable

Test Conditions: Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. The calculation used an estimated Log Kow of 4.33 (estimated using a C10 structure with double bonds in 5 locations).

Results

Value(mg/L) at temperature (°C): 5.2 mg/L (25°C)

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

Flag: Key study for SIDS endpoint

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

EPIWIN (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: CAS No. 25339-53-1, Decene

Method

Method: ISO 2719

GLP: No data

Results

Value: 45°C

Type of test: Closed cup [X]; Open cup []; Other []

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

Reference:

Remark: IUCLID cites Shell Chemicals UK Ltd, Chester

2.8 Auto Flammability (Solids/Gases)

No data available

2.9 Flammability

No data available

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. 25339-53-1, Decene; or CAS No. 872-05-9, 1-Decene

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:	<p>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.</p> <p>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.</p> <p>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.</p> <p>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).</p> <p>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).</p> <p>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.</p>
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. 25339-53-1, Decene or CAS No. 872-05-9, 1-Decene

Method

**Method/
guideline followed:** Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan and Howard (1993). Program used the structure for 1-decene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser (type): OH
Rate Constant: 35.83 E-12 cm³/molecule-sec
Degradation % after: 50% after 3.582 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 22.92 hrs (using avg. OH conc. of 7 E11 mol/cm³) 35.8302

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 (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental

B. Stability in Water

Test Substance

Identity: CAS No. 25339-53-1, Decene; or CAS No. 872-05-9, 1-Decene

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 decene or 1-decene.

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

Data not available

3.2 Monitoring Data (Environment)

Data not available

3.3 Transport and Distribution

3.3.1 Transport between environmental compartments

A. Test Substance

Identity: CAS No. 25339-53-1, Decene

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: 140
Water solubility: 0.329 g/m³
Vapor pressure: 279 Pa (25°C)
Log Kow: 5.70
Melting point: -45.48°C
Environment name: EQC Standard Environment

Half-life in air = 5.59 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	98.1%	1.32%
Water	<1%	19.3%
Soil	1.82%	36.3%
Sediment	<1%	43.0%

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

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

Reliability: (2) Valid with restrictions: 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. 872-05-9, 1-Decene

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: 140
Water solubility: 0.57 g/m³
Vapor pressure: 223 Pa (25°C)
Log Kow: 5.70
Melting point: -66.3°C
Environment name: EQC Standard Environment

Half-life in air = 5.59 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	96.1%	1.11%
Water	<1%	17.9%
Soil	3.85%	41.1%
Sediment	<1%	39.9%

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

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

Reliability: (2) Valid with restrictions: 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.

C. Test Substance

Identity: CAS No. 25339-53-1, Decene or CAS No. 872-05-9, 1-Decene

Method

Type: Volatilization from water

Remarks: Calculated using the computer program EPIWIN version 3.10; based on Henry's Law Constant of 2.68 atm-m³/mole (HENRY experimental database).

Results: Half-life from a model river: 1.209 hrs
Half-life from a model lake: 4.7 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.

D Test Substance

Identity: 5-decene

Method

Media: air – biota – sediment – soil - water
Method: calculation according to MacKay, Level I
GLP: Not applicable

Results

Value:
Air: 99.8%
Water: 0.1%
Soil/sediment: 0.1%

Reliability: (2) Reliable with restrictions: These data were calculated.

Reference: MacKay, D., Multimedia Environmental Models: The Fugacity Approach. Lewis Publishers Inc. Chelsea Michigan USA, 1991.

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

E. Test Substance

Identity: 5-decene

Method

Type: adsorption
Remarks: Based on a calculated KOC (6666 l/kg) for 5-decene
Media: water - soil

Results

Conclusions: Substance is expected to be insignificantly mobile in soil.

Reliability: (2) Reliable with restrictions: These data were calculated.

References: Swann, R.L., D.A. Laskowshi, P.J. McCall, K. Vander-Kuy and H.J. Dishburger (1983) A rapid method for the estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio and water solubility. Residue Reviews 85:17-28.

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

F. Test Substance

Identity: 5-decene

Method

Type: volatility
Media: water - air

Results: Based on a calculated Henry's Law constant for 5-decene the volatilization half-life of the substance in a model river, depth 1 m and current 1 m/s and a wind velocity of 3 m/s is estimated to be 3.5 hours.

Reliability: (2) Reliable with restrictions: These data were calculated.

References: Lyman, WJ et al.. (1982). Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, Chapter 15.

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

3.3.2 Distribution

A. Test Substance

Identity: CAS No. 25339-53-1, Decene or CAS No. 872-05-9, 1-Decene

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 the structure for 1-decene.

Results

Value: Estimated Koc = 1724

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: 5-decene

Method: calculated Koc (soil partition coefficient)

Type: adsorption

Conditions: Brigg's Correlation : $\log Koc = 0.52 \log Kow + 0.88$ assuming $\log Kow = 7$

Media: water-soil

Results

Value: Koc = 33,175

Reliability: (2) Reliable with restrictions: These data were calculated.

References: ENICHEM, Environmental partitioning model: a computer program prepared by Garlanda T and Mascero Garlanda M. (1990).

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

C. Test Substance

Identity: CAS No. 25339-53-1, Decene or CAS No. 872-05-9, 1-Decene

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 values of VP = 209 mm Hg and WS = 0.329 mg/L. Program used the structure for 1-decene.

Results

Value: Bond estimate = 1.11 atm-m³/mole
Group estimate = 2.13 atm-m³/mole
VP/Wsol estimate = 1.17 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.

D. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

Method: No data

Test Conditions: No data

Results

Value: Henry's Law Constant = 2.68 atm-m³/mole at 25°C

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

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.

3.4 Aerobic Biodegradation

A. **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103 PQ11)

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/guideline: EEC Directive 84/449/EEC; Similar to OECD (301 D) Closed Bottle Test.

Test Type: aerobic

GLP: Yes

Year: 1984

Contact time: 28 days

Innoculum: activated sludge

Test Conditions: Microorganisms were obtained from Sittingbourne Sewage Works (UK) and prepared according to standard test protocols. C10-13 Alpha Olefin was added to the test medium from a stock solution containing 2.4 g/L emulsified in Dobane PT sulphonate. The final test concentration was 2 mg olefins 103/L. Test bottles were incubated at 21±1°C and the extent of biodegradation was determined by measuring oxygen concentration in the bottles at days 5, 15 and 28. Controls with no microbial inoculum (control) and with medium plus microbial inoculum only (blank) were included. Sodium benzoate was used as a biodegradable substance to demonstrate the activity of the microbial inoculum.

Results: Under these test conditions, 103 PQ11Olefin was oxidized to 40% of the theoretical oxygen demand by day 5 and 65-70% by day 28 with no lag period. There was no significant inhibition of microbial activity under the test conditions. The report indicated that 103 Olefin was considered readily biodegradable; however, insufficient information was available to determine whether the 10-day window criterion was satisfied.

Reliability: (2) Reliable with restrictions: No information on kinetic of biodegradation or biodegradation of reference substance.

References: Miller RC, Watkinson RJ. (1984). Olefins 103 PQ 11: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center (unpublished report).

B. Test Substance

Identity: C10-13 (Shop Olefins 103), internal

Remarks: Blend of linear olefins: CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method

Method/guideline: OECD 301D Closed Bottle Test

Type: Aerobic [X] Anaerobic []

GLP: Yes

Year: 1985

Contact time: 28 days

Inoculum: Activated domestic sludge

Test Conditions: Microorganisms were obtained from Sittingbourne Sewage Works (UK) and prepared according to standard test protocols. C10-13 Olefin was added to the test medium from a stock solution containing 2.4 g/L emulsified in Dobane PT sulphonate. The final test concentration was 2 mg olefins 103/L. Test bottles were incubated at 21±1°C and the extent

of biodegradation was determined by measuring oxygen concentration in the bottles at days 5, 15 and 28. Controls with no microbial inoculum (control) and with medium plus microbial inoculum only (blank) were included. Sodium benzoate was used as a biodegradable substance to demonstrate the activity of the microbial inoculum.

Results: Under these test conditions, 103 Olefin was oxidized to 54% of the theoretical oxygen demand by day 5 and 60-67% by day 28 with no lag period. 89% of the possible oxygen demand had been consumed in the bottles titrated on day 15. Based on the 15-day results, the 10-day window criterion for "readily biodegradable" appears to have been met; however, the lower values found on day 28 confound the evaluation.

Reliability: (2) Reliable with restrictions: No information on kinetic of biodegradation or biodegradation of reference substance.

Reference: Turner, S.J., Watkinson, R.J., (1985) Shop Olefins 103: An assessment of Ready Biodegradability, Sittingbourne, Shell Research Limited, SBGR.85.106 (unpublished report).

C. Test Substance

Identity: CAS No. 68526-56-7; Alkenes, C9-11, C10 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 42 mg/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 21% 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	20.9, 19.9, 22.6	21.1
Na Benzoate	98.9, 95.5	97.2

* replicate data

Reliability: (1) Reliable without restriction

Flag: Key study for SIDS endpoint

Reference: Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119294A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

D. Test Substance

Identity: CAS No. 872-05-9, 1-Decene

Method

Method/guideline: Manometric respirometry (OECD 301F)

Type: Aerobic [X] Anaerobic []

GLP: Yes

Year: 1995

Contact time: 28 days

Inoculum: Domestic activated sludge

Test Conditions: No data

Results: Degradation = 80.9% after 28 days

Remarks: Concentration = 18.6 mg/L related to test substance. 10 day time window = day 3 to day 13; degradation at the end of the 10 day time window = 64.9% (mean); degradation at plateau = 81% (mean).

Reliability: (2) Reliable with restrictions. Specific test conditions were not reported; however, the test was conducted under GLPs and using a current OECD

test guideline. The report was reviewed for the Alpha Olefins SIAR and the decene dossier approved at SIAM 11.

Reference: Enichem Instituto G Donegani (1995) Final report on ready biodegradability (manometric-respirometric) of olefin C10 (unpublished report).

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

E. Test Substance

Identity: CAS No. 25339-53-1, Decene

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

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

3.5 BOD5, COD or ratio BOD5/COD

No data available

3.6 Bioaccumulation

Test Substance

Identity: CAS No. 25339-53-1, Decene or CAS No. 872-05-9, 1-Decene

Method

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

Test Conditions: Based on chemical structure and an experimental Log Kow of 5.70 from the EPIWIN database, using methods described by Meylan et al., 1999. Formula used to make BCF estimate: $\text{Log BCF} = 0.77 \text{ log Kow} - 0.70 + \text{correction (alkyl chains [8+ -CH}_2\text{- groups] with a value of -1)}$.

Results

Value: Estimated Log BCF = 2.689 (BCF = 488.7)

Reliability: (2) Reliable with restrictions: Results are 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

Sewage Treatment

Test Substance

Identity: CAS No. 25339-53-1, Decene

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility. Input values: MW = 140.27; Henry's LC = 2.68 atm-m³/mol; air-water partition coefficient = 109.604; Log Kow = 5.7; biomass to water partition coefficient = 100,238; temperature = 25°C

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results: 99.89 % 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. 68526-56-7; Alkenes, C9-11, C10 Rich

Method

Method/guideline: OECD 203
Test type: Semistatic 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: 0.2, 0.4, 1.2, 3.5, and 10 mg/L, which measured 0.01, 0.03, 0.06, 0.08, and 2.6 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 0.03 mg/L.

Water hardness was 160-180 mg/L as CaCO₃. Test temperature was 16C (sd = 0.2). Lighting was 445 to 555 Lux with a 16-hr light and 8-hr dark

cycle. Dissolved oxygen ranged from 8.7 to 9.9 mg/L for "new" solutions and 7.2 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.3 to 8.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.175 g; mean total length at test termination = 3.0 cm; test loading = 0.19 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 = 4.8 mg/L (95% CI 3.8 to 6.0 mg/L) based upon loading rates.
96-hour LC50 = 0.12 mg/L (95% CI 0.11 to 0.14 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
0.2	0.01	0
0.4	0.03	0
1.2	0.06	0
3.5	0.08	3
10	0.26	15**

* 15 fish added at test initiation
** 1 mortality not test related

Reliability: (1) Reliable without restriction

Flag: Key study for SIDS endpoint

References: Exxon Biomedical Sciences, Inc. (1996) Fish, Acute Toxicity Test. Study #119258. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

B. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 internal olefins)

Remarks: Blend of linear olefins: CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Semi-static Fish Acute Toxicity Test
GLP: Not stated
Year (study performed): 1984
Species: Rainbow Trout (*Salmo gairdneri*)
Analytical Monitoring: No
Exposure Period: 96 Hours
Statistical Method: Visual inspection

Test Conditions: Control and dilution water was laboratory mains tap water obtained from bore holes in the chalk of North Downs (U.K.). Water was dechlorinated and passed through particle and activated carbon filters (alkalinity 253 mg/L as CaCO₃, hardness 274 mg/L as CaCO₃, conductivity 510 µS/cm, pH 7.3). Test vessels were glass aquaria each filled with 10 L of water and contained 10 fish per vessel. Quantities of test substance were added directly to six aquaria to give concentrations of 20, 50, 100, 200, 500, and 1000 mg/L. The seventh aquarium served as a control and received no test substance. The fish were not fed during the test. Test fish had a mean length of 3.0 cm (range 2.5 to 3.3 cm) and a mean weight of 0.23 g (range 0.15 to 0.32 g). Fingerlings were obtained from Itchen Valley Trout Farm, Alresford, Hampshire, U.K. and acclimated to test conditions for more than 10 days before use. One replicate per treatment and control was used. The aquaria were gently aerated to maintain dissolved oxygen concentration. At 24 h intervals, the number of dead fish was recorded and any dead removed, dissolved oxygen and pH were measured in the old and fresh solutions of the control and high concentration, and the test solutions were renewed. Temperature in one test aquarium was monitored at 4h intervals throughout the test. Total hardness was determined in each batch of fresh media. Test temperature was 13-17 Deg C. Dissolved oxygen ranged from 10.0 to 10.4 mg/L in the fresh media and 9.8 to 10.2 mg/L in the old solutions. pH was 8.2 – 8.4. Total hardness was 240-260 mg/L as CaCO₃. Photoperiod was not stated in the test report.

Results:

Units/Value: 96h LL0 =1000 mg/L; LC50 > solubility

Remarks: Observations made during the study suggest the test substance was not wholly soluble at concentrations of approximately 20 mg/L and greater as indicated by an oily film visible on the surface of the test solutions. Concentrations were expressed as the amount of test substance added. No fish died during the 96h exposure in the 1000 mg/L treatment. The 96h LC50 was > solubility. There were also 100% survival in the control, 50, 100, 200 and 500 mg/L treatments. One fish died (10% mortality) in the 20 mg/L treatment. Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (2) Reliable with restrictions. Test substance was not wholly soluble at the concentrations tested. A more appropriate and currently accepted

method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*. Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

C. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Semi-static Fish Acute Toxicity Test

GLP: Not stated

Year (study performed): 1985

Species: Rainbow Trout (*Salmo gairdneri*)

Analytical Monitoring: No

Exposure Period: 96 Hours

Statistical Method: Visual inspection

Test Conditions: Control and dilution water was laboratory mains tap water obtained from bore holes in the chalk of North Downs (U.K.). Water was dechlorinated and passed through particle and activated carbon filters (alkalinity 255 mg/L as CaCO₃, hardness 270 mg/L as CaCO₃, conductivity 545 µS/cm, pH 7.4). Test vessels were glass aquaria each filled with 10 L of water and contained 10 fish per vessel. Quantities of test substance were added directly to two aquaria to give concentrations of 500 and 1000 mg/L. A third aquarium served as a control and received no test substance. The fish were not fed during the test. Test fish had a mean length of 4.1 cm (range 3.9 to 4.5 cm) and a mean weight of 0.66 g (range 0.47 to 0.86 g). Fingerlings were obtained from Itchen Valley Trout Farm, Alresford, Hampshire, U.K. and acclimated to test conditions for more than 10 days before use. One replicate per treatment and control was used. The aquaria were gently aerated to maintain dissolved oxygen concentration. At 24 h intervals, the number of dead fish was recorded and any dead removed, dissolved oxygen and pH were measured in the old and fresh solutions of the control and high concentration, and the test solutions were renewed. Temperature in one test aquarium was monitored at 4h

intervals throughout the test. Total hardness was determined in each batch of fresh media. Test temperature was 18.5 ± 1.0 Deg C. Dissolved oxygen ranged from 9.6 to 10.2 mg/L in the fresh media and 9.0 to 9.8 mg/L in the old solutions. pH was 7.4 – 8.4. Total hardness was 222-262 mg/L as CaCO_3 . Photoperiod was not stated in the test report.

Results:

Units/Value: 96h LC50 was > solubility; LL0 = 1000 mg/L

Remarks: The test substance was not wholly soluble at the test concentrations and was visible as floating droplets. Concentrations were expressed as the amount of test substance added. Only one fish died during the 96h exposure in the 1000 mg/L treatment. The 96h LC50 was > solubility. There was 100% survival in the control and 500 mg/L treatment.

Reliability:

(3) Reliable with restrictions. Test substance was not wholly soluble at the concentrations tested. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only two concentrations were tested, 2) only one replicate per concentration was used, and 3) analytical verification of the test substance in the exposure solutions was not performed.

Reference:

Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficient. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

Other:

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

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

A. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 linear ninternal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Static Daphnid Acute Toxicity Test

GLP: Not stated

Year (study performed): 1983
Species: Water Flea (*Daphnia magna*)
Analytical Monitoring: No
Exposure Period: 48 hours
Statistical Method: Probit analysis

Test Conditions: Nominal loading rates in the definitive test were 0, 0.05, 0.1, 0.2, 0.5, 1, 2, and 5 mg/L. Control and dilution water was reconstituted hard water prepared by adding salts to glass-distilled deionized water following EPA guidelines (hardness 170 mg/L as CaCO₃). Quantities of stock solutions of the test substance in acetone were added to triplicate sets of 140 ml conical flasks and made up to 140ml with dilution water. Three flasks served as controls and received no test substance. Acetone concentration in control and test flasks was 0.1 ml/L. Ten daphnids, less than 24h old, were placed in each flask. Daphnids were obtained from laboratory cultures and collected from cultures aged between 15 and 35 days. Young for testing were not taken from cultures containing adults with ephippia. In order to minimize daphnids from potentially being trapped in undissolved test substance at the surface of the test solutions, loosely fitting black paper caps were placed over the flasks to create a darkened zone which the daphnids would avoid. After 24 and 48h, the numbers of immobilized daphnids were recorded. Temperature in one test vessel was monitored at 4h intervals. The pH and dissolved oxygen concentration in a control and highest treatment were determined at test initiation and termination. Total hardness of the dilution water used was measured at the beginning of the test. Test temperature was 18 – 22 Deg C. Photoperiod was 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.8 to 9.2 mg/L. pH was 8.0 – 8.3. Total hardness of the water was 170 mg/L as CaCO₃.

Results:

Units/Value: 48-h EL50 = 0.74 mg/L (nominal)

Remarks No undissolved test substance was observed even at 5 mg/L, the highest concentration tested.. Concentrations were expressed as the amount of test substance added. 48-h EL50 = 0.74 mg/L (nominal)with 95% confidence limits of 0.61-0.88 mg/L. There was no immobilization of *D. magna* in the control, 0.05, and 0.1mg/L after 48-h. There were 1 (3.3%), 7 (23.3%), 19 (63.3%), 30 (100%) and 30 (100%) daphnids immobilized in the 0.2, 0.5, 1, 2, and 5 mg/L, respectively. Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (2) Reliable with restrictions. This study was well documented and comparable to a guideline study. Information provided indicate that test concentrations did not appear to have exceeded water solubility of the test substance as evidenced by absence of undissolved material in the exposure solutions. However, analytical verification of the test substance in the test solutions was not performed.

Flag: Key study for SIDS endpoint

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*. Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

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

B. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Static Daphnid Acute Toxicity Test

GLP: Yes

Year (study performed): 1985

Species: Water Flea (*Daphnia magna*)

Analytical Monitoring: No

Exposure Period: 48 hours

Statistical Method: Probit analysis

Test Conditions: Nominal loading rates in the definitive test were 0, 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460 and 1000 mg/L. Control and dilution water was reconstituted hard water prepared by adding salts to glass-distilled deionized water following EPA guidelines (hardness 168-169 mg/L as CaCO₃). Before use, a soil extract was added to the reconstituted fresh water at 20 ml/L. The soil extract was prepared by autoclaving 100 g soil/L distilled water for 15 min at 120 deg C and filtered through Whatman GF/C filter. Quantities of stock solutions of the test substance in Analar acetone were added to triplicate sets of 140 ml glass flasks and made up to 140ml with dilution water. Three flasks served as controls and received no test substance. Acetone concentration in control and test flasks was 0.1 ml/L. Ten daphnids, less than 24h old, were placed in each flask. Daphnids were obtained from laboratory cultures and collected from cultures aged between 15 and 35 days. Young for testing were not taken from cultures containing adults with ephippia. In order to minimize daphnids being trapped in the surface layer of test substance visible at all test concentrations, loosely fitting black caps were placed over the flasks to create a darkened zone which the daphnids would avoid. After 24 and 48h, the numbers of immobilized daphnids were recorded. Temperature in one test vessel was monitored at 4h intervals. The pH and dissolved oxygen concentration in a control and highest treatment were determined

at test initiation and termination. Total hardness of the dilution water used was measured at the beginning of the test. Test temperature was 18 – 22 Deg C. Photoperiod was 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.6 to 9.0 mg/L. pH was 8.0 – 8.4. Total hardness of the water was 170 mg/L as CaCO₃.

Results:

Units/Value: 48-h EL50 = 480 mg/L (nominal)

Remarks: The test substance was not wholly soluble at all test concentrations and was visible at the surface. Concentrations were expressed as the amount of test substance added. 48-h EL50 = 480 mg/L with 95% confidence limits of 400-580 mg/L. There was no immobilization of *D. magna* in the control, 1.0, 2.2, 4.6, 10, 22, 46 and 100 mg/L after 48-h. There were 3 (10%), 14 (46.7%), and 27 (90%) daphnids immobilized in the 220, 460, and 1000 mg/L, respectively.

Reliability: (3) Not Reliable. Test substance was not wholly soluble at the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Analytical verification of the test substance in the exposure solutions was also not performed.

Reference: Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficient. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

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

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

A. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Algal Toxicity Test

GLP: Not stated

Year (study performed): 1983
 Species: Freshwater Green Alga (*Selenastrum capricornutum*)
 Analytical Monitoring: No
 Exposure Period: 4 days
 Statistical Method: EL50 values determined by probit analysis

Test Conditions: Control and dilution water was algal nutrient medium prepared by dissolving Analar grade salts in glass-distilled deionized water according to EPA guidelines except that boric acid was present at 105 µg/L and sodium bicarbonate at 50 mg/L. Sixteen Erlenmeyer flasks containing 50 ml of culture medium were prepared. Quantities of stock solutions of the test substance in acetone were added to ten flasks to give concentrations of 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg/L. Six flasks served as controls and received no test substance. Acetone concentration in the control and treatment flasks was 0.1 ml/L. Each flask was inoculated with algal cells to yield an initial concentration of 500 cells/ml. Algal cells were obtained from laboratory cultures that were originally derived from a strain from American Type Culture Collection (ATCC 22662). Flasks were incubated in a cooled orbital (100 cycles/min) incubator under constant illumination (~3000 lux) at 22-26 deg C (monitored at 4h intervals). After 2 and 4 days incubation, cell counts were made using a Coulter Counter. The initial pH in the control and highest concentration was 7.9 – 8.0. The 96h EC50 (concentration causing a 50% reduction in cell number at day 4 compared to mean control cell number at day 4) was calculated using log transformed concentration values.

Results:

Units/Value: 96h EL50 based on cell numbers at day 4 was 24 mg/L

Remarks: The test substance was not wholly soluble at concentrations of approximately 20 mg/L and greater as indicated by an oily film visible on the surface of the test solutions. Concentrations were expressed as the amount of test substance added. The 96h EC50 based on cell numbers at day 4 was 24 mg/L with 95% confidence limits of 2.9-79 mg/L).

Nominal Conc. (mg/L)	Day 4 Cell Conc. (cells/ml x 10 ⁶)	Day 4 cell number as % Day 4 mean control cell number
Control	1.03(mean)	
1.0	1.1	112
2.2	1.1	110
4.6	1.1	108
10	0.87	85
22	0.33	32
46	0.092	9
100	0.13	13
220	0.11	11
460	0.093	9
1000	0.096	9

Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (3) Not Reliable. Test substance was not wholly soluble at some of the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*. Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

B. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Algal Toxicity Test

GLP: Yes

Year (study performed): 1985

Species: Freshwater Green Alga (*Selenastrum capricornutum*)

Analytical Monitoring: No

Exposure Period: 4 days

Statistical Method: EC50 values determined by probit analysis

Test Conditions: Control and dilution water was algal nutrient medium prepared by dissolving Analar grade salts in glass-distilled deionized water according to EPA guidelines except that boric acid was present at 105 µg/L and sodium bicarbonate at 50 mg/L. Sixteen Erlenmeyer flasks containing 50 ml of culture medium were prepared. Quantities of stock solutions of the test substance in Analar acetone were added to ten flasks to give concentrations of 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg/L. Six flasks served as controls and received no test substance. Acetone concentration in the control and treatment flasks was 0.1 ml/L. Each flask was inoculated with algal cells to yield an initial concentration of 500 cells/ml. Algal cells were obtained from laboratory cultures that were originally derived from a strain from American Type Culture Collection (ATCC 22662). Flasks were incubated in a cooled orbital (100 cycles/min) incubator under constant illumination (~3000 lux) at

22.0-26.5 deg C (monitored at 4h intervals). After 2 and 4 days incubation, cell counts were made using a Coulter Counter. The pH in the control and highest concentration ranged from 7.4 – 7.6 at test initiation and 7.1 – 7.4 at test termination. The 96h EC50 (concentration causing a 50% reduction in cell number at day 4 compared to mean control cell number at day 4) was calculated using log transformed concentration values.

Results:

Units/Value: 96h EL50 based on cell numbers at day 4 was 22 mg/L

Remarks: The test substance was not wholly soluble at 220, 460, and 1000 mg/L and was visible as floating droplets which precluded cell counting. Concentrations were expressed as the amount of test substance added. The 96h EL50 based on cell numbers at day 4 was 22 mg/L with 95% confidence limits of 19-24 mg/L).

<u>Nominal Conc. (mg/L)</u>	<u>Day 4 Cell Conc. (cells/ml x 10⁶)</u>	<u>Day 4 cell number as % Day 4 mean control cell number</u>
Control	1.25(mean)	
1.0	1.4	115
2.2	1.1	92
4.6	1.4	111
10	1.1	87
22	0.63	51
46	0.12	10
100	0.015	1

Reliability: (3) Not Reliable. Test substance was not wholly soluble at some of the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri*, *Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficient. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

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

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

A. Test Substance

Identity: CAS No. 85535-87-1, Alkenes C10-13, linear internal olefins

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method

Method: Inhibition of growth

GLP: No data

Species: *Pseudomonas fluorescens*

Exposure Period: No data

Analytical Monitoring: No data

Results: Maximum inhibition was 19% at 1000 mg/L

Reliability: (4) Not assignable

Reference: Turner, S.J., Watkinson, R.J., (1985) Shop Olefins 103: An assessment of Ready Biodegradability, Sittingbourne, Shell Research Limited, SBGR.85.106 (unpublished report).

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

B. Test Substance

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

Method

Method: Acute static bioassay

GLP: No

Type: Aquatic

Species: Thirteen marine bacteria

Exposure Period: 16 hours

Analytical Monitoring: No data

Test Conditions: Water samples collected from Cleveland and Victoria Point on the Brisbane coast, southeastern Queensland, Australia, were cultured on marine salts medium solidified with 1.5% agar. Thirteen different marine bacteria were isolated and transferred to new media. This culture was maintained at 30°C and subcultured weekly. The test articles were dissolved in ethanol and added to media (maximum 0.1 ml in 50 ml). 0.1 mg of bacterial culture containing 8×10^{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. 25339-53-1, Decene ; CAS No. 872-05-9, 1-Decene; or CAS No. 68526-56-7, Alkenes, C9-11, C10 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 Kow values of 5.12 for decene and 1-decene, and 4.69 for Alkenes, C9-11, C10 Rich. The Kow values were estimated by EPIWIN using the structure for 1-decene for decene and 1-decene; and a structure with double bonds in 3 locations for the C10 Rich substance.

Results:

Units/Value: Estimated 30-day ChV for decene = 26 µg/L
Estimated 30-day ChV for 1-decene = 26 µg/L
Estimated 30-day ChV for Alkenes C9-11, C10 Rich = 59 µg/L

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

(1) **Test Substance:** CAS No. 872-05-9, 1-Decene

Method/Guideline: OECD Guideline 211

Year (guideline): 1998

Type (test type): Daphnid Chronic Toxicity Test

GLP (Y/N): Yes

Year (study performed): 2004

Species: *Daphnia magna* Straus

Analytical Monitoring: Yes

Exposure Period: 21 days

Statistical Method: The EC10 and EC50 values were calculated using the Power Model of the Benchmark Dose (BMD) method (USEPA, 2001). The LOEC and NOEC was determined using the Wilcoxon Rank Sum (Hollander and Wolfe, 1999) with Bonferroni Adjustment (Bland, 1995) using TOXSTAT software (Gulley, 1994). TOXSTAT was also used to perform a t-test with Bonferroni Adjustment (Bland, 1995) to analyze the growth data. United States Environmental Protection Agency (USEPA), Benchmark Dose software, V1.3.1. 2001. Hollander, M. and Wolfe, D.A., Nonparametric Statistical Methods 2nd Ed, John Wiley and Sons, New York, 1999. Gulley, DD and WEST, Inc. TOXSTAT, V.3.4. Western Ecosystems Technology, Inc. Cheyenne, WY, 1994.

Bland, MJ., "Multiple significance tests: the Bonferroni method", British Medical Journal, v310, pg. 170, 1995.

Test Conditions:

1-Decene in a closed system was aerated using an air stone at an air flow rate of 160 to 180 cc/min. The vapor generated from the aeration procedure flowed into an aspirator bottle and bubbled through vehicle/dilution medium (reconstituted water). The 1-decene saturated vapor passed through an air stone near the bottom of the aspirator bottle providing maximum contact between the test substance in the vapor phase and vehicle/dilution medium. This procedure was followed to develop a stock solution, which was diluted to achieve a range of exposure solutions.

The test chambers were 125 mL capacity clear glass bottles with foil lined screw tops (no headspace). One daphnid was added to each of 10 replicates. The *Daphnia* were cultured in-house, were <24 hours old, and were from 16-day old parents. The test was performed using a static daily renewal of exposure solutions. Observations for abnormal or immobilized daphnids and neonates were made on each replicate at approximately 24-hour intervals.

Test organisms were fed daily when solutions were renewed by adding 0.4 mL of a 1.3E8 cells/mL suspension of *Pseudokirchneriella subcapitata* to provide approximately 4.2E5 cells/mL. Test organisms were also fed during renewals with 0.05 mL of a 2.5 g/L Microfeast PZ-20 suspension. The feeding rate supplied approximately 0.1 mgC/adult daphnid/day.

Mean test temperature was 20.6°C (S.D. = 0.2) and diurnal light was approximately 16 hours light and 8 hours dark with 16 to 19 $\mu\text{E}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ during full daylight periods. Dissolved oxygen ranged from 7.8 to 9.4 mg/L and pH ranged from 8.0 to 8.4 during the study. Water hardness was 150 mg/L as CaCO₃. The TOC of the dilution water was 0.5127 ppm.

The analytical method used was static headspace GC-FID (HS GC-FID). The methods practical quantitation limit (PQL) is approximately 0.12 ng/mL ($\mu\text{g/L}$) and corresponds to the concentration of the lowest analyzed analytical standard.

Results:

Units/Value:

Effect Concentration (EC10 and EC50) based on reproduction:

	EC10	EC50
21 day	20.0 $\mu\text{g/L}$ (16.2 $\mu\text{g/L}$ *)	28.1 $\mu\text{g/L}$ (27.2 $\mu\text{g/L}$ *)

* 95% Lower Confidence Interval

The LOEC was 28.7 $\mu\text{g/L}$, the highest concentration tested. The NOEC was 19.4 $\mu\text{g/L}$. The LOEC and NOEC are based on reproduction and growth. The NOEC based on mortality was 28.7 $\mu\text{g/L}$, the highest concentration tested.

The control daphnids released their first brood on days 8 and 10. The coefficient of variation for control fecundity was 8.7%.

The following are the endpoint results for the control and exposure solutions.

Nominal Conc. ($\mu\text{g/L}$)	Measured Conc.** ($\mu\text{g/L}$)	Adult Mortality %	Neonates per Adult	Adult Avg. Length (mm)
Control	0	0	153	5.8
10	5.91	10	151	5.6
16	8.74	10	155	5.8
25	12.8	10	138	5.6
40	19.4	0	140	5.6
60	28.7	10	68	5.2

** Average of new and old solutions (3 replicates each) sampled on day 0 & 1, 7 & 8; 14 & 15, 20 & 21. The sample size for each concentration was $n = 24$, except for the $5.91 \mu\text{g/L}$ concentration, the sample size was $n = 23$. One sample was not used. It was noted that the stock container outlet was not purged, resulting in a spurious value. The table below shows the new and old range of concentrations.

Nominal Conc. ($\mu\text{g/L}$)	Measured Conc. new solutions ($\mu\text{g/L}$)	Measured Conc. old solutions ($\mu\text{g/L}$)
Control	0	0
10	8.15 - 18.4	0.06†
16	13.6 - 24.0	0.06† - 0.126
25	21.3 - 30.2	0.06† - 0.160
40	30.6 - 48.2	0.06† - 0.211
60	44.5 - 68.0	0.06† - 0.477

† 1-decene not detected above Practical Quantitation Limit (PQL= $0.12 \mu\text{g/L}$). PQL X 0.5 ($0.06 \mu\text{g/L}$) used in place of < PQL.

The maximum water solubility of 1-decene under the conditions used to generate the stock solution for this study was approximately $210 \mu\text{g/L}$.

Conclusion: The 1-decene *Daphnia magna* 21 day EC10 was $20.0 \mu\text{g/L}$ and the EC50 was $28.1 \mu\text{g/L}$. Reproduction and growth were more sensitive than survival, resulting in an NOEC of $19.4 \mu\text{g/L}$ and an LOEC of $28.7 \mu\text{g/L}$.

Flag: Key study for SIDS endpoint

Reliability: (1) Reliable without restriction.

Reference: ExxonMobil Biomedical Sciences, Inc. (2004). *Daphnia magna* Reproduction Test with 1-DECENE. Study # 180446. Performed at ExxonMobil Biomedical Sciences, Inc. Annandale, NJ.

Other (source): Higher Olefins Panel, American Chemistry Council

(2) **Test Substance:** CAS No. 25339-53-1, Decene; CAS No. 872-05-9, 1-Decene; or CAS No. 68526-56-7; Alkenes, C9-11, C10 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 Kow values of 5.12 for decene and 1-decene, and 4.69 for Alkenes, C9-11, C10 Rich. The Kow values were estimated by EPIWIN using the structure for 1-decene for decene and 1-decene; and a structure with double bonds in 3 locations for the C10 Rich substance.

Results:

Units/Value: Estimated 16-day EC50 = 32 µg/L
Estimated 16-day EC50 = 32 µg/L
Estimated 16-day EC50 = 64 µg/L

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. 25339-53-1, Decene ; CAS No. 872-05-9, 1-Decene; or CAS No. 68526-56-7; Alkenes, C9-11, C10 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 Kow values of 5.12 for decene and 1-decene, and 4.69 for Alkenes, C9-11, C10 Rich. The Kow values were estimated by EPIWIN using the structure for 1-decene for decene and 1-decene; and a structure with double bonds in 3 locations for the C10 Rich substance.

Results:

Units/Value: Estimated 96-hr ChV = 73 µg/L
Estimated 96-hr ChV = 73 µg/L
Estimated 96-hr ChV = 133 µg/L

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

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 $\mu\text{mol/kg}$, in organs from 1 – 500 $\mu\text{mol/kg}$ and in fat from 5 – 10000 $\mu\text{mol/kg}$. In blood and organs, the detection limits generally were within the range from 0.1 to 1 $\mu\text{mol/kg}$; in fat from 1 to 10 $\mu\text{mol/kg}$.

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-C10 1-alkenes and iso-alkanes in the rat after repeated exposures. *Pharmacology & Toxicology* 73:163-168.

5.2 Acute Toxicity

A. Acute oral toxicity

(1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103 PQ11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline: NA
Type (test type): LD50
GLP: Pre-GLP
Year: 1977
Species/Strain: Rat/Wistar
Sex: Males and females
No. of animals per sex per dose: 4
Vehicle: none
Route of administration: Oral gavage

Test Conditions: Male and female rats, aged approximately 12 weeks, were used at each dose level (5 and 10 ml/kg). The animals were weighed, fasted overnight and the calculated dose of material administered by intraesophageal intubation using a ball point needle fitted to a syringe. After dosing food and water were freely available throughout a 9 day observation period.

Results:

Value: LD50 > 7740 mg/kg

Number of deaths at each dose level: 1 at 10 ml/kg

Remarks: Animals showed no signs of toxic reaction during the 9 day observation period. One female rat died following a period of not eating and drinking and loss of body weight. Under the conditions of this study, C10-13 Olefins have a low order of toxicity.

Reliability: (1) Reliable without restrictions.

Flag: Key study for SIDS endpoint

References: Shell Toxicology Laboratory, Tunstall (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11 (unpublished report).

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

(2) **Test Substance**

Identity (purity): CAS No. 872-05-9, 1-Decene

Method

Method/guideline: No data

Type (test type): LD50

GLP: No

Year: 1973

Species/Strain: Rat /strain not mentioned

Sex: No data

No. of animals per

sex per dose: No data

Vehicle: NA

Route of administration: Oral gavage

Test Conditions: Single treatment dose level of 10g/kg.

Results:

Value: LD50 > 10 g/kg
Number of deaths at each dose level: None
Remarks: No signs of toxicity
Reliability: (2) Reliable with restrictions: Incomplete reporting
Flag: Key study for SIDS endpoint
References: Ethyl Corporation (1990) Internal data (unpublished report).
Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

B. Acute inhalation toxicity

(1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103), linear
Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)
Method
Method/guideline: 4-hr exposures in a dynamic exposure system.
Type (test type): LC50
GLP: No
Year: 1980
Species/Strain: Rat/Wistar
Sex: Males and females
No. of animals per sex per dose: 5
Vehicle: None
Route of administration: Inhalation (mist)
Test Conditions: One group of 10 rats each (5 males and 5 females, approximately 10 weeks of age) was exposed for 4 hrs to a saturated concentration of test substance (> 2.1 mg/L; ~ 305 ppm). Animals were observed for 14 days post-exposure. Initial, 7 day and 14 day body weights were recorded.

The animals were contained within 7 liter glass chambers fitted with carriers to accommodate five animals each, through which

the test atmosphere was passed at a minimal rate of 10 liters/minute.

The test atmosphere was generated by flash vaporization of the test substance supplied to a heated flask by means of a micro metering pump. The vapor was blended with dilution air in a mixing flask, and the vapor/air mixture was passed through an air cooled condenser and a condensation trap to the inhalation chambers. Continuous analysis of the atmosphere during exposure was undertaken using a heated total hydrocarbon analyzer.

Results:

Value: LC50 >2.1 mg/L (~305 ppm) (saturated concentration) mist.

Number of deaths at each dose level: None

Remarks: Some rats lachrymated and salivated during exposure, but no other toxic signs were observed during the 14 day observation period.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Blair, D., Sedgewick, A.E. (1980) The acute inhalation toxicity of Olefins 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.80.052 (unpublished report).

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

(2) **Test Substance:** CAS No. 872-05-9, 1-Decene

Method

Method/guideline: 1 and 4-hr exposures

Type (*test type*): LC50

GLP: No

Year:

Species/Strain: Rat/Sprague Dawley

Sex: No data

No. of animals per sex per dose: No data

Vehicle: None

Route of administration: Inhalation

Test Conditions: Exposures at saturation of 9.3 and 8.7 mg/L (g/m^3) (1621 and 1516 ppm); 14 observation period

Results:

Value: LC50 > saturation concentration

Number of deaths at each dose level: None

Remarks: No visible pathological changes seen after 14 days.

Reliability: (2) Reliable with restrictions: Incomplete reporting

Flag: Key study for SIDS endpoint

References: Ethyl Corporation (1990) Internal data (unpublished report).

Other: This study was included in the dossiers for 1-decene at SIAM 11.

C. Acute dermal toxicity

(1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline: Noakes and Sanderson

Type (test type): LD50

GLP: Pre-GLP

Year: 1977

Species/Strain: Rat/ Wistar

Sex: Males and females

No. of animals per sex per dose: 4

Vehicle: NA

Route of administration: Dermal

Test Conditions: Groups of animals, aged 12-13 weeks, were exposed to the test substance in single exposures to concentrations of 1, 2, and 4 ml/kg. Undiluted test material was applied to shorn dorso-lumbar skin and bandaged into contact with the skin using an impermeable dressing of aluminium foil and water proof plaster. Following the 24-hour exposure period, the dressings were removed and the exposed area was sponged with tepid dilute

detergent solution to remove residue. Animals were observed for gross signs of toxicity daily for 9 days.

Results:

Value: LD₅₀ > 3080 mg/kg

Number of deaths at each dose level: 4 mortalities occurred in the female rats at dose level 4 ml/kg; one each at day 6 and day 8, 2 at day 7.

Remarks: Rats showed no signs of toxic reactions, but those that eventually died did not eat or drink and lost body weight. On the basis of these figures, the acute percutaneous LD50 was estimated to be greater than 4 ml/kg (3080 mg/kg) in males and between 2 and 4 ml/kg (between 1540 and 3080 mg/kg) in females.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Shell Toxicology Laboratory, Tunstall (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11 (unpublished report).

(2) **Test Substance**

Identity (purity): CAS No. 872-05-9, 1-Decene

Method

Method/guideline: U.S. Federal Hazardous Substances Labeling Act

Type (test type): LD50

GLP: Pre-GLP

Year: 1967

Species/Strain: Albino rabbits

Sex: Males

No. of animals per sex per dose: 4

Vehicle: NA

Route of administration: Dermal

Test Conditions: Two groups of 4 rabbits (weighing between 2.3 and 3.0 kg) were used (treated and control). Prior to dosing, the animals were clipped free of hair over the entire trunk area. The skin of two animals from each group was abraded by making longitudinal epidermal abrasions spaced about 2-3 cm apart over the area to be exposed. Surgical gauze was wrapped around the animal and

covered with an impervious plastic film. The animals in the treated group then received a dose of 10 g/kg test substance introduced under the plastic film. Following dosing, the animals were immobilized in stocks for 24 hr, after which the covering and excess material were removed and the skin examined for gross changes. Animals were weighed on Days 1-4, and on Days 7 and 14. Animals were observed for 14 days and then sacrificed and autopsied.

Results:

Value: LD₅₀ > 10 g/kg
Number of deaths at each dose level: No mortalities that were related to exposure to test substance. One control animal died from pneumonia on Day 2.

Remarks: There were no signs suggestive of systemic toxicity. The skins of animals became very taut, dry and scaly, with no regrowth of hair in the clipped areas and a loss of hair from areas which became wet with the test substance. Autopsy showed no gross signs of damage to internal organs. Slight signs of pneumonia were observed in both treated and control animals. All treated animals showed weight loss on Days 1-7:

	% Weight Loss					
	Day 1	Day 2	Day 3	Day 4	Day 7	Day 14
1-Decene	-4	-10	-10	-9	-6	+1
Control	0	+2	+2	+3	+1	+4

Reliability: (2) Reliable with restrictions: Details of procedures are not available, individual animal data is not available, and animals appeared to have pneumonia.

Flag: Key study for SIDS endpoint

Reference: Rinehart, W.E. (1967) Toxicological Studies on Several Alpha Olefins, for Gulf Research and Development Company (unpublished report).

Other: This study was included in the dossier for 1-decene 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. 872-05-9, 1-Decene, 100%, NEODENE® 10 Alpha Olefin

Method: TSCA Health Effects Test Guidelines, 40 CFR 798.4470, meeting OECD Guidelines, Section 404

Test Type: in vivo
GLP: Yes
Year: 1995

Test Conditions

Species: Rabbits
Strain: New Zealand White
Cell type:
Sex: Male and female
Number of animals per sex per dose: 3
Total dose: 0.5 ml
Vehicle: None
Exposure time period: 4 hrs
Grading scale: Draize

Method Remarks: A 0.5 ml quantity of undiluted test material was applied onto a 1 inch by 1 inch gauze square. The test material was applied in this manner to the shaved dorsal skin at one intact site on each of six rabbits and occluded with rubber dental dam throughout the 4 hour exposure period. Severe irritation persisted 72 hours following application. All six animals were held for a Day 7 reading. The values for each rabbit were totaled and averaged for erythema and eschar formation at ½ to 1 hour, 24 hours, 48 hours, and 72 hours. The values for edema were evaluated at ½ to 1 hour, 24, 48, and 72 hours.

Results: There were no deaths during the study. By day 7 reading, all irritation had cleared in two animals, while the remaining four animals exhibited slight to severe irritation. The only change noted in the coloration and/or texture of the skin was desquamation. No evidence of corrosion (necrosis) was found. The Draize Primary Dermal Irritation Index (the mean of combined scores for erythema and edema at 1 hour, 24 hour, 48 hour and 72 hour) was calculated to be 5.3.

Reliability: (1) Reliable without restrictions

Reference: Hilltop Biolabs, Inc. (1992) Primary Skin Irritation Study in Rabbits; Performed for Shell Oil Company (unpublished report).

(2) **Test Substance:** CAS No. 872-05-9, 1-Decene (GULFTENE 10)

pH: Not applicable

Method: OECD 404

Test Type: in vivo

GLP: Yes

Year: 1995

Test Conditions

Species: Rabbits

Strain: New Zealand White

Cell type:

Sex: Male and female

Number of animals per sex per dose: 5 males and 1 female

Total dose: 0.5 ml

Vehicle: None

Exposure time period: 4 hrs

Grading scale: Draize

Method Remarks: At the start of the study, the animals weighed 2.37 to 2.76 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: All animals gained weight during the study. Exposure produced well-defined erythema and very slight to moderate oedema that cleared by Day 14. 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 3.67. The mean 24-72 hr scores for erythema and edema were 2.0 and 1.7, respectively.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 10, Report 703/077. Conducted by Safepharma Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

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

B. Eye Irritation/Corrosion

(1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

pH: Not applicable

Method:

Test Type: in vivo
GLP: No
Year: 1977

Test Conditions

Species: Albino rabbits
Strain: New Zealand White
Number of animals per dose: 4

Dose(s) used: 0.2 ml
Vehicle: None
Observation period: 7 days

Remarks: The conjunctival redness chemosis and discharge, corneal opacity and damage to the iris following the instillation of 0.2 ml undiluted olefin into the conjunctival sac of four rabbit eyes was scored using standard Draize scales.

Results: Animals were observed within 1-2 hours, after 1, 2, 3, and 7 days of application. Mean Draize score was 1.0 (out of 110) at 1 hour after exposure, 0.9 for day 1, 0.1 for day 2, and 0 at other points.

Reliability: (1) Reliable without restrictions

Reference: Cassidy, S.L., Clark, D.G. (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.0.171.77 (unpublished report).

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

(2) **Test Substance:** CAS No. 872-05-9, 1-Decene

pH: Not applicable

Method: equivalent to OECD 405

Test Type: in vivo

GLP: No

Year: 1967

Test Conditions

Species: Albino rabbits

Strain: Not specified

Cell type:

Sex: Males

Number of animals per dose: 6

Dose(s) used: 0.1 ml

Vehicle: None

Observation period: 72 hrs

Scoring method used: Draize scoring at 24, 48, and 72 hours after treatment

Remarks: A positive control group were exposed to 5% Ivory Soap solution

Results: Draize score at 24 hours was 0.7/110; 0.3 at 48 hours and 0.0 at 72 hours. Maximum individual score = 2/110 at 24 and 48 hours. The mean 24-72 hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis, respectively, were 0, 0, 0.2, and 0.

Reliability: (1) Reliable without restrictions

Reference: Rinehart, W.E. (1967) Toxicological Studies of Several Alpha Olefins Conducted by Department of Occupational Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania, for Gulf Research and Development Company (unpublished report).

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

(3) **Test Substance:** CAS No. 872-05-9, 1-Decene

pH: Not applicable

Method: No data
Test Type: in vivo
GLP: No
Year: 1973

Test Conditions

Species: Rabbit
Strain: New Zealand White
Number of animals per dose: No data

Dose(s) used: No data
Vehicle: None
Observation period: 72 hrs

Results: Non-irritating.

Remarks: All scores = 0 at 24 and 72 hrs

Reliability: (1) Reliable without restrictions

Reference: Ethyl Corporation (1990) internal data (unpublished report).

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

5.4 Skin Sensitisation

Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method: Magnusson and Kligman
Test Type: challenge
GLP: No
Year: 1977

Test Conditions

Species: Guinea pig
Strain: P strain
Sex: Male and female
Number of animals per sex per dose: 10 in test group; 5 each in control group

Route of administration: Injection and Topical

Intradermal
 Induction conc.: 0.05%
 Induction vehicle: corn oil

Topical
 Induction conc.: 1.5%
 Induction vehicle: corn oil
 Challenge conc.: 10%
 Challenge vehicle: corn oil

Method remarks: A preliminary screen was carried out using groups of 2 male and 2 female guinea pigs to determine the concentrations of test material to be used for intradermal induction, topical induction and topical challenge.

Induction was accomplished in 2 stages, intradermal injection and a topical application. Two rows of 3 injections were made: 2 of 0.1 ml Freund's complete adjuvant (FCA), 2 of 0.1 ml test material in solvent (solvent), and 2 of 0.1 ml test material in 50:50 FCA/solvent. The injection sites were just within the boundary of a 4x4 cm shaved area.

One week after the intradermal injections the same area was clipped. A 4x4 cm patch of Whatman No. 3 filter paper was soaked in a solution of the test material, placed over the injection sites of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm). This was secured with elastic adhesive bandage (Poroplast). The dressing was left in place for 48 hours.

The challenge procedure was carried out 2 weeks after topical induction. Challenge was accomplished by topical application of the challenge solution of the test material to the flank of both test and control groups of animals. 3x3 cm area on the flank was clipped and shaved. A 2.5x2.5 cm patch of Whatman No. 3 filter paper was soaked in a solution of the test material, placed over the injection sites of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm). This was secured with elastic adhesive bandage (Poroplast). The dressing was left in place for 24 hours. Examination of the challenge site was immediately, 24 and 48 hours after removal of the dressing.

Results: Negative for sensitization

Results Remarks: Number of animals with skin reaction at challenge: 0/10
 Number of animals with skin reaction in control group at challenge: 0/10.

Reliability: (1) Reliable without restrictions

Reference: Cassidy, S.L., Clark, D.G. (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.0.171.77 (unpublished report).

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

5.5 Repeated Dose Toxicity

No data available

5.6 Genetic Toxicity *in vitro*

A. Gene Mutation

- (1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103), linear
- Remarks:** Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline: in-vitro bacterial reverse mutation – Ames Assay

Type: bacterial

System of testing: bacterial

GLP: No

Year: 1983

Species/Strain: *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP₂ or WP₂ uvrA

Metabolic activation: With and without S9 fraction from induced rat livers

Concentrations tested: 31.25, 62.5, 125, 250, 500, 1000, 2000 and 4000 µg/plate

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

Test Conditions: 20 µl volumes of solutions of Olefin 103 PQ/11 in ethanol/Tween 80 (1.5625, 3.125, 6.25, 12.5, 50, 100 mg/ml) or 40 µl of 100 mg/ml were added to top agar mix to give final solutions of 31.25, 62.5, 125, 250, 500, 1000, 2000 and 4000 µg/plate both in the presence and in the absence of rat liver S9 fractions. The cultures were incubated at 37°C for 48-72 hours before the revertant colonies were counted. The activity of the S9 mix and the sensitivities of the strains TA1538, TA98 and TA100 were monitored by treating cultures with a known positive control compound, benzo (a) pyrene, which requires metabolic activation before it is able to induce gene mutation. The sensitivity of TA1537 was monitored by the indirect mutagen, neutral red; the sensitivities of *E. coli* WP₂ or WP₂ uvrA pkm 101 and TA1535 were monitored by testing with the direct-acting mutagens, potassium dichromate or sodium azide, respectively.

Results

Cytotoxic conc.: No cytotoxicity observed
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material did not lead to an increase in reverse mutation frequency in any strain. No visible precipitation of the test compound was observed in the top agar overlay. Microscopic examination of the background lawn in the plate incorporation assay showed no reduction in growth in any of the strains tested. All positive and negative controls responded in a manner consistent with data from previous assays. The addition of Olefin 103 PQ/11 at amount up to 4000 µg per plate to agar layer cultures of *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP₂ or WP₂ uvrA did not lead to an increase in the reverse gene mutation frequency in any of the strains either in the presence or absence of rat liver S9 fractions.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint.

References: Brooks, TM, Clare, MG, Wiggins, DE (1983) Toxicity studies with detergents: Genotoxicity studies with Olefin 103 PQ/11 (Cracked Urea Wax Olefin). Shell Research Limited, SBGR.83.299 (unpublished report).

(2) **Test Substance:** CAS No. 872-05-9, 1-Decene (manufactured by Schuchard)

Method

Method/guideline: OECD 471
Type: in-vitro bacterial reverse mutation – Ames Assay
System of testing: bacterial
GLP: Yes
Year:
Species/Strain: *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538 without S9 ; and TA98 and TA100 with S9
Metabolic activation: With and without S9 fraction as noted above
Concentrations tested: No data
Statistical Methods: No data

Test Conditions: No data

Results

Cytotoxic conc.: Toxicity seen in TA100 and TA1538 without S9
Genotoxic effects: Negative with and without metabolic activation

Reliability: (2) Reliable with restrictions: Data were not reviewed for quality but were reviewed for SIAM 11.

References: Burghardtova, K. , B. Horvathova and M. Valachova (1984) Testing of some 1-alkenes by the method of Ames. Biologia (Bratislava), vol. 39(11):1121-1125 (in Czech.) (unpublished report).

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

B. Chromosomal Aberration

Test Substance: C10-13 Internal Olefins (Shop Olefins 103), linear

Remarks: Blend of CAS No. 25339-53-1 (C₁₀ = 6-12%); CAS No. 28761-27-5 (C₁₁ = 27-45%); CAS No. 25378-22-7 (C₁₂ = 37-47%); CAS No. 25377-82-6 (C₁₃ = 8-17%)

Method

Method/guideline:
Type: in-vitro rat liver cell chromosome aberration assay
System of testing: non-bacterial
GLP: No
Year: 1983
Type of cell used: Rat liver RL1 cells
Metabolic activation: No
Concentrations tested: up to 500 µg/ml
Statistical Methods:

Test Conditions: The range of concentrations of the test compound to be used to assess the cloning efficiency was determined from the results of the initial assay. For each concentration, including the solvent control, three 9 cm diameter Petri dishes were used. Five hundred RL4 cells were added to each dish and cells were incubated in 10 ml tissue culture medium at 37°C in a humidified atmosphere containing 5% CO₂. Twenty-four hours after adding the cells, the medium was replaced with medium containing the compound or solvent, which was replaced with fresh medium after 24 hours exposure. Five days later the cells were fixed and stained. Colonies containing at least 50 cells were counted. The concentration of the test compound that reduced the number of colonies to an average of approximately 50% of those on the dishes exposed to solvent only was used as the highest concentration in the chromosome assay.

Results

Cytotoxic conc.: No cytotoxicity observed
Genotoxic effects: Negative

Remarks: There was no significant increase in the frequency of chromatid gaps, chromatid breaks or total chromatid aberrations in rat liver (RL4) cell cultures exposed to Olefin 103 PQ/11 at concentrations up to 25 ug per ml. All positive and negative controls responded in a manner consistent with data from previous assays.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Dean, B.J. (1980) Toxicity studies with detergent intermediates: In vitro genotoxicity studies with Shop process components. Shell Research Limited, TLGR.80.074 (unpublished report).

5.7 Genetic Toxicity *in vivo*

No data available

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 C₃ 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-decene at SIAM 11.

5.11 Experience with Human Exposure

No data available

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