

201-15013B

# HPV Data Set

## EP-290

# Robust Summaries

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**Existing Chemical Memo CAS No.** : ID: 68526-82-9  
: Alkenes,C6-10, hydroformylation products, high boiling  
: 68526-82-9

**Producer related part**  
**Company** : BASF Corporation  
**Creation date** : 11.11.2002

**Substance related part**  
**Company** : BASF Corporation  
**Creation date** : 11.11.2002

**Status Memo** : Prepared by  
Elmer Rauckman PhD DABT  
Toxicology and Regulatory Affairs  
Freiburg IL 62243  
618-539-5280  
rauckman@toxicsolutions.com

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**Chapter (profile)** :  
**Reliability (profile)** :  
**Flags (profile)** :

# 1. General Information

Id 68526-82-9  
Date 30.12.2003

## 1.0.1 APPLICANT AND COMPANY INFORMATION

Type : manufacturer  
Name : BASF Corporation  
Contact person :  
Date :  
Street : 3000 Continental Drive  
Town : Mt. Olive, NJ 07828-1234  
Country :  
Phone :  
Telefax :  
Telex :  
Cedex :  
Email :  
Homepage :

16.12.2003

## 1.2 SYNONYMS AND TRADENAMES

## 2. Physico-Chemical Data

Id 68526-82-9  
Date 30.12.2003

### 2.1 MELTING POINT

**Value** : ca. -44 °C  
**Method** : Determined by an unknown method by BASF Corporation on product.  
**Test substance** : EP-290 Heavy Oxo Ends BASF Product number 526251  
**Reliability** : (2) valid with restrictions  
26.10.2003 (29)

### 2.2 BOILING POINT

**Value** : ca. 130 - 273 °C at 13 hPa  
**Decomposition** :  
**Method** : other: distillation control  
**Year** :  
**GLP** :  
**Test substance** :  
**Remark** : This range represents the initial boiling point of the mixture to the boiling point after 80% of the product has been removed. A certain percent of residue would also remain.  
**Test substance** : EP-290 Heavy Oxo Ends BASF Product number 526251  
**Reliability** : (2) valid with restrictions  
26.10.2003 (29)

### 2.3 DENSITY

**Type** : density  
**Value** : = .845 g/cm<sup>3</sup> at 20 °C  
**Remark** : This is a measured value for typical product  
**Test substance** : EP-290 Heavy Oxo Ends BASF Product number 526251  
**Reliability** : (2) valid with restrictions  
26.10.2003 (29)

### 2.4 VAPOUR PRESSURE

**Value** : < .01 hPa at 25 °C  
**Decomposition** :  
**Method** : other (calculated)  
**Year** :  
**GLP** :  
**Test substance** :  
**Method** : EPIWIN 3.05 was used to determine the vapor pressures of several typical components to gain an understanding of the components probable vapor pressure range.

## 2. Physico-Chemical Data

Id 68526-82-9

Date 30.12.2003

**Result** : Structures were input using standard SMILES notation.

Component	Vapor Pressure (mm Hg)		Higher VP(hPa)
	Exp*	Calc	
n-C9 alcohol	0.023	0.033	0.044
n-C11 alcohol	0.003	0.005	0.007
n-C13 alcohol	0.0004	0.0002	0.0003
n-C20 alcohol	0.00000005	0.0000001	0.00000013
C9 Diether (C18)	0.000053	0.0007	0.0009
1-Hexedecene (C16)	0.0026	0.0077	0.01
C11-C11 Ester (C22)	--	0.00019	0.0003

\* Experimental vapor pressures as found in the SRC database contained in EPIWIN.

**Test substance** : Representative model compounds

**Conclusion** : Most components are of very low volatility and have a vapor pressure below 0.01 hPa

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

EPIWIN estimates are assigned a reliability of 2

27.10.2003 (31)

**Value** : = .0035 hPa at 25 °C

**Decomposition Method** :

**Year** :

**GLP** :

**Test substance** : other TS

**Remark** : Most volatile alkene component

**Test substance** : 1-HEXADECENE (CASNO 629-73-2)

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

27.10.2003 (11)

### 2.5 PARTITION COEFFICIENT

**Partition coefficient** : octanol-water

**Log pow** : ca. 3 - 12 at 20 °C

**pH value** : -

**Method** : other (calculated)

**Year** :

**GLP** :

**Test substance** :

**Method** :

Calculation with EPIWIN

The Ko/w of each component (and isomer) was calculated with EPIWIN based on the SMILES notation. The relative quantity of each was used to construct a weighted average for the composite Ko/w. The utility of the composite Ko/w is questionable since the materials will distribute and interact with biological systems independently. The chart showing the entire range of Ko/w values provides an overview of the possible behavior of the components.

## 2. Physico-Chemical Data

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Result	Component	SMILES	log Kow	fract	Rel %
	C9	CCCCCCCCO	3.2965	0.6	2
		CCCCCCC(C)CO	3.223	0.2	
		CCC(CC)CCCCO	3.223	0.15	
		CCC(CC)CC(C)CO	3.1495	0.05	
	C11	CCCCCCCCCO	4.2787	0.6	12
		CCCCCCCC(C)CO	4.2052	0.2	
		CCC(CC)CCCCCO	4.2052	0.15	
		CCC(CC)CCCC(C)CO	4.1317	0.05	
	C13	CCCCCCCCCCCCO	5.2609	0.6	15
		CCCCCCCCCCCC(C)CO	5.1874	0.2	
		CCCCC(CC)CCCCCO	5.1874	0.15	
		CCCCC(CC)CCCC(C)CO	5.1139	0.05	
	C20	CCCCCCCCCCCCCCCCCO	8.6986	0.6	15
		CCCCCCCCCCCCCCCC(C)CO	8.6251	0.2	
		CCCCC(CC)CCCCCCCCCO	8.6251	0.15	
		CCCCC(CC)CCCCCCCC(C)CO	8.5516	0.05	
	C25	CCCCCCCCCCCCCCCCCCCCCO	11.1541		2
	Ethers				
	C18	CCCCCCCCOCCCCCCCC	7.9246		3.5
	C22	CCCCCCCCCOCCCCCCCC	9.889		3.5
	Hexedecene	CCCCCCCCCCCCC=C	8.0626		7.5
	Eicosene	CCCCCCCCCCCCCCCCC=C	9.0448		7
	2-Bu-octol	CCCCCCC(CCCC)CO	4.6963		6.5
	Ester C22	CCCCCCCCCCC(=O)OCCCCCCCC	9.704		2.5
	Ester C28	CCCCCCCCCCCCC(=O)OCCCCCCCCCCCC	11.6684		2.5

Using the weighted average the log  $K_{ow}$  = 7.07

<b>Test substance</b>	:	Representative model compounds	
<b>Conclusion</b>	:	Major components have a Log Kow between about 3 and 12	
<b>Reliability</b>	:	(2) valid with restrictions	
<b>Flag</b>	:	EPIWIN estimates are assigned a reliability of 2	
27.10.2003	:	Critical study for SIDS endpoint	(31)
<b>Partition coefficient</b>	:	octanol-water	
<b>Log pow</b>	:	= 4.11 at 25 °C	
<b>pH value</b>	:		
<b>Method</b>	:		
<b>Year</b>	:		
<b>GLP</b>	:		
<b>Test substance</b>	:	other TS	
<b>Remark</b>	:	Most prevalent single alcohol	
<b>Test substance</b>	:	1-DECANOL (CASNO 112-30-1)	
<b>Reliability</b>	:	(2) valid with restrictions	
12.11.2002	:	Calculated by acceptable method	(25)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water

## 2. Physico-Chemical Data

Id 68526-82-9

Date 30.12.2003

**Value** : < 100 mg/l at 20 °C  
**pH value** :  
**concentration** : at °C  
**Temperature effects** :  
**Examine different pol.** :  
**pKa** : at 25 °C  
**Description** :  
**Stable** :  
**Deg. product** :  
**Method** : other: Calculated  
**Year** :  
**GLP** :  
**Test substance** :

**Method** : EPIWIN 3.05 was used to determine the water solubility of several typical components to gain an understanding of the components range of water solubilities.

**Result** : Structures were input using standard SMILES notation.

Component	Water Sol (mg/L)	
	Exp*	Calc
n-C9 alcohol	140	157
n-C11 alcohol		43
n-C13 alcohol		4.5
n-C20 alcohol		0.002
C9 Diether (C18)		0.0031
1-Hexedecene (C16)		0.001
C11-C11 Ester (C22)		0.00004

\* Experimental value found in SRC data base contained in EPIWIN 3.05

**Test substance** :  
**Conclusion** : Representative model compounds

The most water soluble components have a water solubility in the range of 100 mg/L. The mixture can be considered essentially insoluble in water.

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

**Flag** : EPIWIN estimates are assigned a reliability of 2  
27.10.2003 : Critical study for SIDS endpoint

(31)

#### 3.1.1 PHOTODEGRADATION

Type : air  
Light source : Sun light  
Light spectrum : nm  
Relative intensity : based on intensity of sunlight

Method :  
Calculated with AOP v1.90 Program based on SMILES structure

Result :  
AOP Output

SMILES : CCCCCCCCCCCCCO  
CHEM :  
MOL FOR: C13 H28 O1  
MOL WT : 200.37

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----  
Hydrogen Abstraction = 19.4675 E-12 cm3/molecule-sec  
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 19.6075 E-12 cm3/molecule-sec  
HALF-LIFE = 0.546 Days (12-hr day; 1.5E6 OH/cm3)  
HALF-LIFE = 6.546 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

SMILES : CCCCCCCCCCCCCCCCCO  
CHEM :  
MOL FOR: C20 H42 O1  
MOL WT : 298.56

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----  
Hydrogen Abstraction = 29.3588 E-12 cm3/molecule-sec  
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 29.4988 E-12 cm3/molecule-sec  
HALF-LIFE = 0.363 Days (12-hr day; 1.5E6 OH/cm3)  
HALF-LIFE = 4.351 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

### 3. Environmental Fate and Pathways

Id 68526-82-9  
Date 30.12.2003

```
SMILES : CCCCCCCCCCCCCC=C
CHEM   :
MOL FOR: C18 H36
MOL WT : 252.49
----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----
Hydrogen Abstraction      = 20.8346 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 26.3000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings   = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 47.1346 E-12 cm3/molecule-sec
HALF-LIFE = 0.227 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 2.723 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION -----
OVERALL OZONE Rate Constant = 1.200000 E-17 cm3/molecule-sec
HALF-LIFE = 0.955 Days (at 7E11 mol/cm3)
HALF-LIFE = 22.920 Hrs

Experimental Database: NO Structure Matches
```

```
SMILES : CCCCCCCCCOCCCCCCCCC
CHEM   :
MOL FOR: C20 H42 O1
MOL WT : 298.56
----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----
Hydrogen Abstraction      = 41.6461 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings   = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 41.6461 E-12 cm3/molecule-sec
HALF-LIFE = 0.257 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 3.082 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION -----
***** NO OZONE REACTION ESTIMATION *****
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
```

```
SMILES : CCCCCCCCCC(=O)CCCCCCCCCCC
CHEM   :
MOL FOR: C26 H52 O2
MOL WT : 396.70
----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----
Hydrogen Abstraction      = 31.6744 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings   = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 31.6744 E-12 cm3/molecule-sec
HALF-LIFE = 0.338 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 4.052 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION -----
***** NO OZONE REACTION ESTIMATION *****
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
```

**Source** :  
**Test substance** : Toxicology and Regulatory Affairs Calculation -2003  
**Reliability** : Representative model compounds  
: (2) valid with restrictions  
Calculated by an acceptable method

**Flag** : Critical study for SIDS endpoint (12)  
30.12.2003

#### 3.1.2 STABILITY IN WATER

**Type** : abiotic  
**t1/2 pH4** : at °C  
**t1/2 pH7** : > 1 year at 25 °C  
**t1/2 pH9** : at °C

**Method** :  
Water stability is estimated using chemical principles and EPIWIN modeling.

Most of the components do not contain a water-reactive or hydrolysable group. The following are considered water stable\* for this reason:

- Olefins
- Aliphatic alcohols
- Aliphatic ethers
- Aliphatic carboxylic acids

The materials that are potentially hydrolysable are;

- Aliphatic esters
- Aliphatic acetals

These were entered into EPIWIN (HYDROWIN v1.67) in an attempt to estimate hydrolysis rates using the following SMILES notations

C-11,11 Ester CCCCCCCCC(=O)OCCCCCCCCC  
C-9,9,9 Acetal CCCCCCCCC(OCCCCCCCC)OCCCCCCCC

**Result** :  
Ref: J.C. Harris. Rate of Hydrolysis in Handbook of Chemical Property Estimation Methods, WJ Lyman ed. ACS publication 1990.

The ester has an estimated Kb of 0.01077 L/mol-sec.  
Estimated half-life for ester:  
pH 8 = 2.0 years  
pH 7 = 20.4 years

The program cannot estimate the hydrolysis rate for acetals. Although acetals are chemically considered more labile than esters, they are not hydrolyzed rapidly at neutral pH\*. In addition, since the acetal is almost completely water insoluble (EPIWIN estimated water solubility 0.00000037 mg/L) it will remain with the organic phase and will not have the opportunity to hydrolyze under conditions where a significant amount of EP-290 is in contact with water. Furthermore, the acetal is a low-level component of EP-290 (2-4%) and its hydrolysis would not be a major factor in the overall water stability of the material.

Relative to hydrolysis of the model ester, limited water solubility (EPIWIN estimate 0.000036 mg/L) would severely limit the access of water to the ester in bulk material.

**Test substance** : \* Ref: K. Peter Vollhardt. Organic Chemistry, WH Freeman and Company, New York 1987, p 640.

**Conclusion** : Representative model compounds

**Reliability** : The product is considered stable in water with a half-life >> 1 year  
(2) valid with restrictions

**Flag** : EPIWIN estimates are assigned a reliability of 2  
27.10.2003 : Critical study for SIDS endpoint

(31)

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

**Type** : fugacity model level III

**Media** : other: water

**Air** : % (Fugacity Model Level I)

**Water** : % (Fugacity Model Level I)

**Soil** : % (Fugacity Model Level I)

**Biota** : % (Fugacity Model Level II/III)

**Soil** : % (Fugacity Model Level II/III)

**Method** :

**Year** :

**Method** :

Because this is a complex mixture, when well mixed into the environment, individual components will distribute according to their individual physiochemical properties. To understand the relative distribution of components it is necessary to look at individual representative components. This was accomplished by selecting a range of materials thought to be most representative of various potentials for distribution. Two alcohols (C13 and C20) were selected as these are components and have differing water-solubility and volatility. One representative olefin (C18), one ether (C20) and one ester (C28) were selected. In the calculation procedure, various isomeric forms were examined and were not found to be greatly different. This selection of materials is considered representative of EP-290.

It was assumed that materials originated in water as this is considered the most likely manner in which EP-290 will enter the environment.

### 3. Environmental Fate and Pathways

Id 68526-82-9  
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#### Result

: Alcohol C13 CCCCCCCCCCCCCO

Level III Fugacity Model (Full-Output):

=====

Chem Name :  
Molecular Wt: 200.37  
Henry's LC : 0.000128 atm-m3/mole (Henrywin program)  
Vapor Press : 0.000237 mm Hg (Mppwin program)  
Liquid VP : 0.000276 mm Hg (super-cooled)  
Melting Pt : 31.7 deg C (Mppwin program)  
Log Kow : 5.26 (Kowwin program)  
Soil Koc : 7.46e+004 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.612	13.1	0
Water	50.6	360	1000
Soil	0.0395	360	0
Sediment	48.8	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.52e-012	153	29	15.3	2.9
Water	6.83e-010	462	240	46.2	24
Soil	3.71e-015	0.361	0	0.0361	0
Sediment	2.06e-010	111	4.62	11.1	0.462

Persistence Time: 474 hr  
Reaction Time: 652 hr  
Advection Time: 1.73e+003 hr  
Percent Reacted: 72.7  
Percent Advected: 27.3

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
Air: 13.09  
Water: 360  
Soil: 360  
Sediment: 1440  
Biowin estimate: 3.215 (weeks)

Advection Times (hr):  
Air: 100  
Water: 1000  
Sediment: 5e+004

\*\*\*\*\*

Alcohol C-20: CCCCCCCCCCCCCCCCCO

Level III Fugacity Model (Full-Output):

=====

Chem Name :  
Molecular Wt: 298.56  
Henry's LC : 0.000929 atm-m3/mole (Henrywin program)  
Vapor Press : 5e-007 mm Hg (Mppwin program)  
Liquid VP : 3.08e-006 mm Hg (super-cooled)  
Melting Pt : 105 deg C (Mppwin program)  
Log Kow : 8.7 (Kowwin program)  
Soil Koc : 2.05e+008 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000623	8.7	0
Water	10.2	360	1000
Soil	0.00198	360	0
Sediment	89.8	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.28e-015	0.663	0.0833	0.0663	0.00833
Water	6.32e-012	261	136	26.1	13.6
Soil	9.28e-019	0.0509	0	0.00509	0
Sediment	1.89e-012	578	24	57.8	2.4

Persistence Time: 1.34e+003 hr  
Reaction Time: 1.59e+003 hr  
Advection Time: 8.36e+003 hr  
Percent Reacted: 84  
Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
Air: 8.702  
Water: 360  
Soil: 360  
Sediment: 1440  
Biowin estimate: 2.998 (weeks)

Advection Times (hr):  
Air: 100  
Water: 1000  
Sediment: 5e+004

### 3. Environmental Fate and Pathways

Id 68526-82-9

Date 30.12.2003

\*\*\*\*\*

C-18 Olefin Octadecene : CCCCCCCCCCCCCCCC=C

Level III Fugacity Model (Full-Output):

=====

Chem Name :  
Molecular Wt: 252.49  
Henry's LC : 10.7 atm-m3/mole (Henrywin program)  
Vapor Press : 0.00261 mm Hg (Mppwin program)  
Liquid VP : 0.0029 mm Hg (super-cooled)  
Melting Pt : 29.6 deg C (Mppwin program)  
Log Kow : 9.04 (Kowwin program)  
Soil Koc : 4.5e+008 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000207	4.4	0
Water	10.1	360	1000
Soil	2.83e-006	360	0
Sediment	89.9	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.68e-015	0.437	0.0277	0.0437	0.00277
Water	3.94e-008	261	136	26.1	13.6
Soil	8.25e-018	7.28e-005	0	7.28e-006	0
Sediment	1.18e-008	579	24	57.9	2.4

Persistence Time: 1.34e+003 hr  
Reaction Time: 1.59e+003 hr  
Advection Time: 8.37e+003 hr  
Percent Reacted: 84  
Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
Air: 4.4  
Water: 360  
Soil: 360  
Sediment: 1440  
Biowin estimate: 2.940 (weeks)

Advection Times (hr):  
Air: 100  
Water: 1000  
Sediment: 5e+004

\*\*\*\*\*

C-20 Ether CCCCCCCCCCCCCCCCCC

Level III Fugacity Model (Full-Output):

=====

Chem Name :  
Molecular Wt: 298.56  
Henry's LC : 0.228 atm-m3/mole (Henrywin program)  
Vapor Press : 0.000107 mm Hg (Mppwin program)  
Liquid VP : 0.000345 mm Hg (super-cooled)  
Melting Pt : 76.4 deg C (Mppwin program)  
Log Kow : 8.91 (Kowwin program)  
Soil Koc : 3.33e+008 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000382	6.16	0
Water	10.1	360	1000
Soil	1.75e-005	360	0
Sediment	89.9	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.17e-015	0.574	0.0511	0.0574	0.00511
Water	9.57e-010	261	136	26.1	13.6
Soil	1.24e-018	0.00045	0	4.5e-005	0
Sediment	2.87e-010	578	24	57.8	2.4

Persistence Time: 1.34e+003 hr  
Reaction Time: 1.59e+003 hr  
Advection Time: 8.37e+003 hr  
Percent Reacted: 84  
Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
Air: 6.163  
Water: 360  
Soil: 360  
Sediment: 1440  
Biowin estimate: 3.127 (weeks)

Advection Times (hr):  
Air: 100  
Water: 1000  
Sediment: 5e+004

\*\*\*\*\*

C-26 Ester: CCCCCCCCCC(=O)CCCCCCCCCCCC  
Level III Fugacity Model (Full-Output):  
=====

Chem Name :  
Molecular Wt: 396.7  
Henry's LC : 0.315 atm-m3/mole (Henrywin program)  
Vapor Press : 9.28e-008 mm Hg (Mppwin program)  
Liquid VP : 1.42e-006 mm Hg (super-cooled)  
Melting Pt : 145 deg C (Mppwin program)  
Log Kow : 11.7 (Kowwin program)  
Soil Koc : 1.92e+011 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	7.59e-007	8.1	0
Water	10.1	360	1000
Soil	4.14e-006	360	0
Sediment	89.9	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.83e-018	0.000869	0.000102	8.69e-005	1.02e-005
Water	1.73e-012	261	136	26.1	13.6
Soil	5.31e-022	0.000107	0	1.07e-005	0
Sediment	5.19e-013	579	24.1	57.9	2.41

Persistence Time: 1.34e+003 hr  
Reaction Time: 1.59e+003 hr  
Advection Time: 8.38e+003 hr  
Percent Reacted: 84  
Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
Air: 8.105  
Water: 360  
Soil: 360  
Sediment: 1440  
Biowin estimate: 3.059 (weeks)

Advection Times (hr):  
Air: 100  
Water: 1000  
Sediment: 5e+004

**Test substance** : Representative model compounds

**Conclusion** : The representative compounds if released into water, will distribute primarily to sediment and water depending on their individual Ko/w values. Except for the shorter chain alcoholic components of EP-290, which may distribute equally between water and sediment, the majority of material is expected to distribute to sediment. This is shown in the following summary table from the Level III calculations.

Component	C#	Distribution (Percent)			
		Air	Water	Soil	Sediment
Alcohol	C13	0.61	50.6	0.04	48.8
Alcohol	C20	0.001	10.2	0.002	89.8
Octadecene	C18	0.0002	10.1	0.000003	89.9
Ether	C20	0.0004	10.1	0.00002	89.9
Ester	C28	0.000001	10.1	0.000004	89.9

**Reliability** : (2) valid with restrictions  
Calculated values are assigned a reliability of 2.

**Flag** : Critical study for SIDS endpoint  
26.10.2003

(9)

### 3.5 BIODEGRADATION

**Type** : aerobic  
**Inoculum** : activated sludge, domestic  
**Concentration** : 42 mg/l related to Test substance  
**Degradation** : = 21 (±) % after 28 day(s)

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**Result** : other: limited biodegradation

**Method** : A Manometric Respirometry Test was preformed according to the OECD-301F test guideline (1992).  
GLP: Yes

**Result** :  
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 sodium benzoate positive control was observed, 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.

Percent degradation of test substance in triplicate flasks was: 20.9%, 19.9%, 22.6% (mean = 21.1%)

**Test condition** :  
Non acclimated activated sludge and test medium were combined before adding test material. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, 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 concentration was approximately 42 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/-1 Deg C.

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

**Test substance** : Alkenes, C9-11, C10 Rich, CASNO 68526-56-7, component of EP-290

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

Assigned 2 because original report not available for review. (14)

20.12.2003

**Type** : aerobic  
**Inoculum** : activated sludge, domestic  
**Concentration** : 57 mg/l related to Test substance related to

**Contact time** :  
**Degradation** : = 58 (±) % after 28 day(s)  
**Result** :

**Method** :  
A Manometric Respirometry Test was preformed according to the OECD-301F test guideline (1992).  
GLP: Yes

**Result** :  
Approximately 58% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on Day 7.

By day 14, >60% biodegradation of the sodium benzoate positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen

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		consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.
		Percent degradation of test substance in triplicate flasks was: 60.1%, 60.7%, 53.7% (mean = 58.1%)
<b>Test condition</b>	:	Non acclimated activated sludge and test medium were combined before adding test material. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, 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 concentration was approximately 57 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/-1 Deg C.
<b>Test substance</b>	:	All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
<b>Reliability</b>	:	Olefin hydroformylation products C11-14 iso, C13 rich (68526-86-3) (2) valid with restrictions
20.12.2003		Assigned 2 because original report not available for review. (15)
<b>Type</b>	:	aerobic
<b>Inoculum</b>	:	activated sludge, domestic
<b>Concentration</b>	:	2 mg/l related to Test substance related to
<b>Contact time</b>	:	
<b>Degradation Result</b>	:	= 71 (±) % after 28 day(s) readily biodegradable
<b>Method</b>	:	OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test" Year: (1981) GLP: no
<b>Test substance</b>	:	Dodecanedioic acid CASNO 693-23-2
<b>Reliability</b>	:	(2) valid with restrictions
20.12.2003		Secondary source, IUCLID value from guideline study, assigned 2 (23)
<b>Type</b>	:	aerobic
<b>Inoculum</b>	:	activated sludge, domestic
<b>Concentration</b>	:	43 mg/l related to Test substance related to
<b>Contact time</b>	:	
<b>Degradation Result</b>	:	= 71 (±) % after 28 day(s) readily biodegradable
<b>Method</b>	:	A Manometric Respirometry Test was performed according to the OECD-301F test guideline (1992).

### 3. Environmental Fate and Pathways

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<b>Remark</b>	:	This mixture of alcohols is derived from an essentially identical hydroformylation reaction as that used to produce EP-290. This mixture of alcohols is a component of EP-290
<b>Result</b>	:	<p>The test material was determined to be readily biodegradable. The half-life was reached by day 11. By day 28, 71.1% degradation of the test material was observed. 10% biodegradation was achieved on day 4. By day 14, &gt;60% biodegradation of positive control was observed, which met 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.</p> <p>Replicate flasks containing test material showed the following percent degradation on day 28: 74.0%, 72.6%, 66.5% (mean = 71.1). The control substance, sodium benzoate, showed a 86% biodegradation on day 28.</p>
<b>Test condition</b>	:	<p>Non acclimated activated sludge and test medium were combined prior to addition of test material. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, 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 concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 44mg/L. Test temperature was 22 +/-1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>
<b>Test substance</b>	:	Olefin hydroformylation products C9-11 iso, C10 rich (68526-85-2)
<b>Reliability</b>	:	(2) valid with restrictions
20.12.2003		Assigned 2 because original report not available for review. (13)
<b>Type</b>	:	aerobic
<b>Inoculum</b>	:	activated sludge, domestic
<b>Concentration</b>	:	2 mg/l related to Test substance related to
<b>Contact time</b>	:	30 day(s)
<b>Degradation</b>	:	= 95 (±) % after 30 day(s)
<b>Result</b>	:	readily biodegradable
<b>Method</b>	:	Directive 84/449/EEC, C.6 "Biotic degradation closed bottle test"
		GLP:no
<b>Test substance</b>	:	2-Ethylhexyl Laurate CASNO 20292-08-4
<b>Reliability</b>	:	(2) valid with restrictions
20.12.2003		Secondary source, IUCLID value from guideline study, assigned 2 (22)
<b>Type</b>	:	aerobic

### 3. Environmental Fate and Pathways

Id 68526-82-9  
Date 30.12.2003

**Inoculum** : activated sludge, non-adapted  
**Concentration** : 2 mg/l related to Test substance  
related to  
**Contact time** :  
**Degradation** : = 85 (±) % after 30 day(s)  
**Result** :  
**Method** :  
Directive 84/449/EEC, C.6 "Biotic degradation closed bottle test"  
**Test substance** :  
Dodecanoic acid CASNO 143-07-7  
**Reliability** : (2) valid with restrictions  
Secondary source, IUCLID value from guideline study, assigned 2  
20.12.2003 (24)

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Type** : static  
**Species** : Lepomis macrochirus (Fish, fresh water)  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**NOEC** : = 1000 measured/nominal  
**LC0** : > 1000 measured/nominal  
**LC50** : > 1000 measured/nominal  
**Limit test** : no  
**Analytical monitoring** : no  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** :

**Method**

: After preliminary tests, 10 fish (bluegill sunfish, mean wt 0.30 g) were exposed to the test material at several closely spaced concentrations. Test containers were 5-gallon glass containers containing 15 liters of laboratory well water. Test material was added directly to the vessels without a carrier solvent. Ten fish were added to each container after the test material had been mixed with the test water for less than 30 minutes

## Conditions were:

Temperature 21-23°C  
 Alkalinity 368 ppm as CaCO<sub>3</sub>  
 Hardness 255 ppm as CaCO<sub>3</sub>  
 Dissolved Oxygen 9.5 ppm  
 pH 8.0 (dilution water)  
 DOC not reported

**Remark**

: Examination of the raw data indicates that the test material was not completely dissolved in the water. "Oil type" droplets were reported on the surface at all test concentrations. This may not be a significant issue with a mixture such as this which has components that vary in solubilities.

**Result**

: Not all of the test material dissolved in the water. It was reported that large-oily droplets remained on the surface of the water for the duration of the test at all concentrations.

In the definitive test, the following results were recorded

Conc (mg/L)	# fish	#dead at			
		24hr	48hr	72hr	96hr
0	10	0	0	0	0
100	10	0	0	0	0
180	10	0	0	0	0
320	10	0	0	0	0
560	10	0	0	0	0
1000	10	0	0	0	0

No adverse effects on fish were reported at any concentration.

Oxygen levels were determined in controls, the lowest and the highest

## 4. Ecotoxicity

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concentrations at 0, 48 and 96 hours and did not differ markedly control staying between 5.7 and 9.5 ppm (the lower DO reading were taken at study termination. Measurement of pH levels were done at the same concentrations and times and was from 8.0 to 8.2 for all measurements

**Test substance** : Heavy Oxo Ends, Monsanto Chemical, CASNO 68526-82-9, Average MW 283.4, clear, yellow to green liquid

**Conclusion** :  
The LC50 for bluegill sunfish under these conditions is greater than 1000 mg/L.

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

**Flag** : Well-documented study conducted under glp-like conditions with quality assurance audits of the data and report.  
26.10.2003 Critical study for SIDS endpoint

(3)

**Type** : Static

**Species** : *Salmo gairdneri* (Fish, estuary, fresh water)

**Exposure period** : 96 hour(s)

**Unit** : mg/l

**NOEC** : = 560 measured/nominal

**LC0** : > 1000 measured/nominal

**LC50** : > 1000 measured/nominal

**Limit test** : No

**Analytical monitoring** : No

**Method** :

**Year** :

**GLP** : No

**Test substance** :

**Method** :

After preliminary tests, 10 fish (rainbow trout, mean wt 0.87 g) were exposed to the test material at several closely spaced concentrations. Test containers were 5-gallon glass containers containing 15 liters of laboratory well water. Test material was added directly to the vessels without a carrier solvent. Ten fish were added to each container after the test material had been mixed with the test water for less than 30 minutes

Conditions were:

Temperature	12-13°C
Alkalinity	368 ppm as CaCO <sub>3</sub>
Hardness	255 ppm as CaCO <sub>3</sub>
Dissolved Oxygen	9.2 ppm
pH	7.8 (dilution water)
DOC	not reported

**Remark** : Examination of the raw data indicates that the test material was not completely dissolved in the water. "Oil type" droplets were reported on the surface at all test concentrations. This may not be a significant issue with a mixture such as this which has components that vary in solubilities.

**Result** : Not all of the test material dissolved in the water. It was reported that large-oily droplets remained on the surface of the water for the duration of the test at all concentrations.

In the definitive test, the following results were recorded

Conc (mg/L)	# fish	#dead at				
		24hr	48hr	72hr	96hr	
0	10	0	0	0	0	
32	10	0	0	0	0	
56	10	0	0	0	0	
100	10	0	0	0	0	
180	10	0	0	0	0	
320	10	0	0	0	0	
560	10	0	0	0	0	
1000	10	0	0	0	0	

Effects on fish were limited to the 1000 mg/L group where a few fish were reported to be resting on the bottom at the 72 and 96 hour observation.

Oxygen levels were determined in controls and the lowest and the two highest concentrations at 0, 48 and 96 hours and was only different from control (8.2 ppm) at the 1000 mg/L level (6.0ppm) at study termination. Measurement of pH levels were done at the same concentrations and times and either 8.0 or 8.1 for all measurements.

**Test substance** : Heavy Oxo Ends, Monsanto Chemical, CASNO 68526-82-9, Average MW 283.4, clear, yellow to green liquid

**Conclusion** : The LC50 for rainbow trout sunfish under these conditions is greater than 1000 mg/L.

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

Well-documented study conducted under glp-like conditions with quality assurance audits of the data and report.

**Flag** : Critical study for SIDS endpoint  
20.10.2003

(4)

#### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

**Type** : static  
**Species** : Daphnia magna (Crustacea)  
**Exposure period** : 48 hour(s)  
**Unit** : mg/l  
**NOEC** : = .1 measured/nominal  
**EC50** : = .17 measured/nominal  
**24 hour EC50** : > 1.6 measured/nominal  
**Limit Test** : no  
**Analytical monitoring** : no

**Method** :

A static toxicity test was conducted in 250 mL beakers which contained 200 mL test solution. The dilution water used in this study was well water from St. Peters, Missouri. For each test concentration, the appropriate amount of the test compound, dissolved in dimethylformamide was pipetted into 1000 mL of dilution water and shaken vigorously for 1 minute. This solution was then divided into three 200 mL aliquots in triplicate beakers to provide appropriate replication. The remaining 400 mL were used for 0-hour DO,

pH, alkalinity and hardness determinations. A control, consisting of the same dilution water and conditions but with no test compound was established. Also, a solvent control was employed which consisted of dilution water and the maximum amount of solvent used in the test concentrations. The amount of solvent used in this test was 0.5 mL dimethylformamide/L (DMF).

Nominal test concentrations were selected based on a rangefinding test. All test vessels were maintained at room temperature. Test solutions were not aerated during the test. Ten daphnids were randomly assigned to each test vessel within 30 minutes after the compound was added for a total of 30 daphnids per concentration.

During this test, the dissolved oxygen concentration, pH, alkalinity, hardness, and temperature of test solutions were monitored at the initiation and termination of the toxicity test in the high, middle, low and control test concentrations.

Statistical methods: In tests where the highest percentage of immobilized daphnids was >65 percent, the computer program of Stephan (1978) which calculates an EC50 by three methods, binomial, moving average, and probit analysis, was used.

**Result**

:

During the 48-hour toxicity test, the pH and dissolved oxygen ranged from 7.6 to 8.5 and 5.3 to 8.6 mg/L, respectively. The average temperature was 21C and the alkalinity and hardness ranged from 198 to 290 mg/L and 232 to 322 mg/L.

Visual inspection of the beakers indicated that the water solubility was not exceeded at any concentrations. Both a control and a solvent control were used in this study. No mortality was observed in either set of control organisms.

Conc (mg/L)	% Immobilized	
	24 h	48 hr
Control	0	0
Solvent Cont	0	0
0.1	0	0
0.2	0	83.3
0.4	0	96.7
0.8	30	100
1.6	40	100

**Test substance**

:

Heavy Oxo Ends, Monsanto Chemical, CASNO 68526-82-9, Average MW 283.4, clear, yellow to green liquid. Lot number 1618258.

**Conclusion**

:

The 48 hours EC50 was 0.17 mg/L with a 95% confidence interval of 0.15 to 0.19 mg/L.

The NOEC was 0.1 mg/L

**Reliability**

:

(1) valid without restriction  
Well-documented, guideline-like study

**Flag**

:

Critical study for SIDS endpoint

23.10.2003

(5)

**4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE**

**4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA**

## 5.1.1 ACUTE ORAL TOXICITY

<b>Type</b>	:	LD50
<b>Value</b>	:	> 15800 mg/kg bw
<b>Species</b>	:	rat
<b>Strain</b>	:	Sprague-Dawley
<b>Sex</b>	:	male/female
<b>Number of animals</b>	:	
<b>Vehicle</b>	:	other: Dosed neat
<b>Doses</b>	:	5010, 7940, 12600 and 15800 mg/kg bw
<b>Method</b>	:	
<b>Year</b>	:	
<b>GLP</b>	:	no
<b>Test substance</b>	:	
<b>Method</b>	:	The undiluted test substance was administered undiluted to Sprague-Dawley rats in increasing dose at fractional log intervals. Treated animals were observed for seven days, survivors were sacrificed and subjected to an examination of the viscera. Body weights were only reported at the time of dosing (presumably used to determine the volume of test material to administer). Rats of each sex were used and all were in an initial weight range of 225 to 270 grams. Dose levels and animals per group are given in the results.
<b>Remark</b>	:	Study conducted in 1971
<b>Result</b>	:	Dose levels and grouping were as follows:  Dose (mg/kg) Animals (M = male, F = female) 5,010 1F 7,940 1M 12,600 1F 15,800 3M and 2F  All animals survived the 7-day observation period. Clinical signs reported were loss of appetite and activity for two to four days following administration. No abnormalities were noted at necropsy.
<b>Test substance</b>	:	Monsanto Heavy Oxo Ends, lot 11.16.71, Monsanto sample #174
<b>Conclusion</b>	:	The Oral LD50 is greater than 15,800 mg/kg in Sprague-Dawley rats of each sex.
<b>Reliability</b>	:	(2) valid with restrictions  Good documentation for an older study. Although animals were sacrificed after seven days rather the currently recommended 14, animals had recovered from the initial signs of toxic effects. In addition, as the dose levels were almost 8 times the currently recommended maximum dose, this study is considered an adequate test of oral toxicity. Procedure is similar to current OECD-423 Acute Toxic Class Method. Downgraded to 2 due to only 7-day observation period.

21.10.2003

(30)

## 5.1.2 ACUTE INHALATION TOXICITY

**Type** : LC50  
**Value** : > 4.9 mg/l  
**Species** : rat  
**Strain** : Crj: CD(SD)  
**Sex** : male/female  
**Number of animals** : 20  
**Vehicle** :  
**Doses** : 1.1 and 4.9 mg/L  
**Exposure time** : 4 hour(s)  
**Method** :  
**Year** :  
**GLP** : yes  
**Test substance** :

**Method** :  
 Groups of 5 Sprague-Dawley CD (Charles River) rats of each sex were exposed to test material for four hours as an aerosol at concentrations of 1.1 or 4.9 mg/L. Aerosol was produced using an air atomizing nozzle running at 19.7 or 20.2 L per minute and 26 psi pressure. Exposures were conducted in 100 l Plexiglas chambers which were monitored gravimetrically using filters at approximately hourly intervals. Particle size distributions were determined at 30 minute intervals using either a Battelle cascade impactor (4.9 mg/L group) or a TSI Model 3000 Aerodynamic particle sizer equipped with a TSI Model 3302 dilutor.

Rats were observed for physical signs before exposure, fifteen minutes after exposure began, and hourly thereafter. After the four-hour exposure, animals were allowed to remain in the chambers for 30 minutes to clear the chambers of test substance. Observations were continued on a once daily basis during the subsequent fourteen day post-exposure period. Body weights were recorded on day 1 before exposure and on days 2, 3, 5, 8, and 15. All rats that died on study or were sacrificed at termination of the study were necropsied.

**Result** :  
 It was determined that the mean gravimetric concentration of test substance aerosol at the high concentration was 4.9 mg/L with a range of 3.3 to 5.9 mg/L and that this aerosol was respirable with a MMAD of 2.6 microns and 91% of particles below 10 microns. The lower concentration group had a mean gravimetric concentration of 1.1 mg/L; however, the impactor data were found to be invalid for technical reasons and a particle size determination was not obtained. As the same nozzle and conditions were used to generate the lower concentration aerosol, it was assumed to be respirable as well.

One 4.9 mg/L group male died three days after the exposure and other rats in this group displayed irregular breathing, closed eyes, and matted coats during exposure. After the exposure period, rats were reported to have increased secretory responses, irregular breathing, matted coat, yellow anogenital area, and material on the coat. Rats exposed at 1.1 mg/L displayed similar signs with a lower incidence of irregular breathing. By the middle of the second post-exposure week, all rats were essentially free signs of toxicity. Body weights of 4.9 mg/L group rats were depressed (loss of bodyweight) on days 2 through 8. The bodyweights of the 1.1 mg/L animals were slightly depressed (loss of bodyweight) on days 2 though 5.

Body weight depression may have been related to treatment. The only necropsy finding considered to be treatment related was hair loss in the 4.9 mg/L group.

**Test substance** : Heavy Oxo Ends, Monsanto Chemical, CASNO 68526-82-9, Average MW 283.4, clear, yellow to green liquid

**Conclusion** :  
The four hour LC50 for Heavy Oxo Ends is greater than 4.9 mg/L. Exposure produced signs of respiratory, eye, and skin irritation at 4.9 and 1.1 mg/1. Clear body weight reduction occurred at the 4.9 mg/L with marginal reduction occurring at 1.1 mg/L, A NOAEL was not identified.

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

**Flag** : Modern guideline-like study under glp with excellent documentation.  
26.10.2003 : Critical study for SIDS endpoint (6)

5.1.3 ACUTE DERMAL TOXICITY

**Type** : LD50  
**Value** : > 7940 mg/kg bw  
**Species** : rabbit  
**Strain** : New Zealand white  
**Sex** : male/female  
**Number of animals** : 4  
**Vehicle** : other: neat application  
**Doses** : 3160, 5010, 7940 mg/kg bw  
**Method** :  
**Year** :  
**GLP** : no  
**Test substance** :

**Method** :  
 The test substance was administered undiluted to the closely-clipped skin of New Zealand white male or female rabbits. The treated areas were covered with plastic that was held in place for 24 hours. Animals were observed for 14 days after treatment, sacrifices and necropsied. Increasing incremental doses were used to minimize animal usage. Animals weighed 2.4 to 2.7 kg at treatment. Body weights were determined 5 days after treatment but not at termination.

**Result** :  
 Dose levels and grouping were as follows:

Dose (mg/kg)	Animals	5-Day BW change
3,160	1M	-0.1 kg
5,010	1F	-0.2 kg
7,940	1M	-0.2 kg
7,940	1F	-0.3 kg

All animals survived the 14-day observation period. Clinical signs reported were loss of appetite and activity for three to seven days following administration. No abnormalities were noted at necropsy.

**Test substance** :  
 Monsanto Heavy Oxo Ends, lot 11.16.71, Monsanto sample #174

**Conclusion** :  
 The Dermal LD50 is greater than 7,940 mg/kg in New-Zealand rabbits of each sex

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

Good documentation for an older study. This study is considered an adequate test of dermal toxicity. Procedure is similar to current OECD-423 Acute Toxic Class Method.

**Flag** : Critical study for SIDS endpoint (30)  
23.10.2003

**5.1.4 ACUTE TOXICITY, OTHER ROUTES**

**5.4 REPEATED DOSE TOXICITY**

**Type** : Sub-chronic  
**Species** : rat  
**Sex** : male/female  
**Strain** : Sprague-Dawley  
**Route of admin.** : inhalation  
**Exposure period** : 13-weeks  
**Frequency of treatm.** : 5 days per week  
**Post exposure period** :  
**Doses** : target 100, 300 and 1000 mg per cubic meter  
**Control group** : yes, concurrent vehicle  
**NOAEL** : = 100 mg/m<sup>3</sup>  
**LOAEL** : = 300 mg/m<sup>3</sup>  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** :

**Method** :  
 Groups of 15 Sprague-Dawley rats of each sex were exposed to atmospheres containing the test substance (TS) six hours a day, five days a week for 13 weeks.

Chambers were one cubic meter steel and glass operated dynamically at calibrated initial airflows between 199 and 218 liters per min. Aerosol was generated from the neat test material using a Laskin nebulizer at backpressures of 5, 8, or 15 psi for low, mid and high dose groups respectively.

The target levels of TS were 0, 100, 300, and 1000 mg/m<sup>3</sup>. Rats were observed twice daily for signs of toxicity and were weighed at weekly intervals. Ophthalmoscopic examinations were conducted prior to the start of treatment and at the end of the study. Blood was obtained from 10 rats/group for evaluation before the study, after about one month of treatment, and at the end of the study. The specific parameters evaluated are listed below. A complete necropsy was performed on all animals that died on test, or were sacrificed at study termination.

The following organs were weighed for all survivors: adrenals, brain, kidneys, liver, lungs, and reproductive organs (ovaries or testes with epididymides).

Hematology parameters examined were:

- hemoglobin
- hematocrit
- erythrocyte count
- platelet count
- total and differential leukocytes
- erythrocyte morphology

Clinical Chemistry parameters examined were

- total serum protein
- albumin
- albumin/globulin ratio
- serum glutamic pyruvic transaminase
- serum glutamic oxaloacetic transaminase
- alkaline phosphatase
- fasting glucose
- cholesterol
- triglycerides
- blood urea nitrogen
- lactic acid dehydrogenase
- creatinine
- uric acid
- total bilirubin
- direct bilirubin
- calcium
- phosphorus
- potassium
- sodium
- chloride

Tissues listed below were examined from rats in the control and high-dose group. The lungs, lymph nodes, and nasal turbinates were also examined in rats from the mid- and high-dose groups.

- abdominal aorta
- adrenals (2)
- bone and bone marrow (sternum)
- brain (three sections including frontal cortex and basal ganglia, parietal cortex and thalamus; cerebellum and pons)
- esophagus
- eyes (2)
- gonads
- ovaries (2) or testes with epididymides (2)
- heart
- intestine
- cecum
- colon
- duodenum
- ileum
- jejunum
- rectum
- kidneys (2)
- liver (2 sections, from separate lobes)
- lungs (each lobe and mainstem bronchi)
- lymph nodes (peribronchial and mesenteric)
- nasopharyngeal tissues (4 sections of head)
- pancreas

- pituitary
- salivary glands (submandibular)
- sciatic nerve
- spleen
- stomach
- thymic region
- thyroid/parathyroid
- trachea
- urinary bladder
- uterus (horns and cervix)

low and mid-dose groups also had the following examined

- lungs
- lymph nodes
- nasal turbinates

**Result**

:

The gravimetrically measured levels of test substance (TS) for groups (male/female) were 105/105, 294/293 and 1014/1009 mg/m<sup>3</sup>. Analysis by a gas chromatographic method confirmed the accuracy of the gravimetric method. An analysis of the particle size distribution indicated that the test material was administered in a respirable aerosol. Impactor analysis showed a MMAD of 1.6, 1.4 or 1.6 microns for low, mid and high dose groups, respectively with 100% of the particles less than 10 micron.

One mid-dose female was accidentally killed during the interim blood sample collection and one high-dose male and two high-dose females died during the study. The high-dose group deaths were considered treatment related. An increased incidence of nasal discharge and rough coats were observed in rats from the mid- and high-dose groups. No treatment related ophthalmoscopic findings were present. Body weights gains were slightly reduced in high-dose rats by about 8% throughout the study. This reduction was statistically significant only for females.

Few statistically significant hematological and clinical chemistry changes were observed and there was no pattern consistent with a treatment related effect; therefore, the following changes were not considered as toxicologically significant. High-dose males at interim sacrifice showed increased erythrocyte counts and serum phosphorus. High-dose males at terminal sacrifice showed increased BUN and decreased triglycerides.

Organ weights: Relative and absolute lung weights were increased for mid-dose males and rats of each sex in the high-dose group. This was associated with an increased incidence of intra-alveolar accumulation of macrophages and considered treatment related. Other changes in organ weights were observed for the mean relative weights of kidneys, adrenals and liver in the high-dose females. None of these were associated with evidence of organ damage or clinical-chemistry associated findings and were, thus, not considered toxicologically significant.

Pathology: A cytoplasmic accumulation of eosinophilic material, ranging from minimal to moderate in severity, was observed in the respiratory epithelial cells of almost all treated rats and a small number of control rats. The severity of this finding indicated a dose response relationship. Treated rats, but not controls, showed minimal to moderately severe necrosis of the respiratory-epithelium that was accompanied by an accumulation of eosinophilic particulate material on the luminal surface of the mucosa.

High-dose group animals showed subacute to chronic interstitial inflammation of mild to moderate severity. An increased intra-alveolar accumulation of macrophages was observed in the lungs of rats from the mid- and high-dose groups. Focal accumulation of foamy macrophages, which ranged in severity from minimal to moderate, was observed in treated rats. Other gross and microscopic changes, which were observed, either occurred in the treated and control rats or they occurred spontaneously.

No changes attributed to treatment in any organ system related to reproductive function were mentioned in the laboratory report although most reproductive organs from high dose and control animals underwent macroscopic and microscopic evaluation.

<b>Test substance</b>	:	Heavy Oxo Ends, Monsanto Chemical, CASNO 68526-82-9, liquid, Lot number 1618277, received by laboratory 9 July 1984.
<b>Conclusion</b>	:	Clear treatment related effects were observed in rats from the high-dose group manifest as reduced body weight gains, increased lung weights and microscopic pulmonary morphology. Mid-dose group animals exhibited an increase in lung weigh only for males and microscopic effects that were considered by the examining pathologist to be indicative of a "physiological response to aerosol exposure" and of questionable toxicological significance. In light of the dose-response continuum and minimal microscopic effects at the low dose, the mid dose is considered a LOAEL and the low dose is considered a NOAEL. The only target organ identified was the respiratory tract.
<b>Reliability</b>	:	(2) valid with restrictions
<b>Flag</b>	:	This is a modern, guideline-like, complete, and well documented study. No glp statement was found in the report. For this reason, the study is assigned a reliability score of 2.
26.10.2003	:	Critical study for SIDS endpoint (2)

## 5.5 GENETIC TOXICITY 'IN VITRO'

<b>Type</b>	:	Ames test
<b>System of testing</b>	:	Reverse mutation, plate incorporation
<b>Test concentration</b>	:	
<b>Cycotoxic concentr.</b>	:	
<b>Metabolic activation</b>	:	with and without
<b>Result</b>	:	negative
<b>Method</b>	:	
<b>Year</b>	:	
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS

<b>Method</b>	:	The mutagenic potential of behenyl alcohol was evaluated using the S. typhimurium strains TA1535, TA1537, TA1538, TA98, and TA100 with and without metabolic activation. The tester strains were exposed to behenyl alcohol according to the direct plate incorporation method. Liver microsomal fractions from 8- to 12-week-old male Wistar rats were prepared according to established methods. Positive controls consisted of sodium azide and 4-nitro-Ophenylenediamine, tested without metabolic
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activation, and aminoanthracene, tested with metabolic activation. Negative controls were untreated or exposed to only solvent. Behenyl alcohol was dissolved in ethanol and tested at concentrations of 10.0, 100.0, 333.3, 666.6, and 1000.0 mg/plate. The selection of doses was based on the results of a previously conducted range-finding study. Assays were performed in two independent experiments, using identical procedures, both with and without metabolic activation. Each concentration, including the controls, was tested in triplicate. The colonies were counted using a BIOTRAN 111 counter connected to a PC.

For a test substance to be considered positive in tester strain TA100, at least a twofold increase was required in the number of reversions. In tester strains TA1535, TA1537, TA1538, and TA98, a test substance was considered positive when the number of reversions was at least three times higher than the spontaneous reversion rate. In addition, a dose-dependent increase in the number of revertants was regarded as an indication of possible mutagenic potential, regardless of whether the highest dose induced a two- to threefold increase in the number of revertants.

**Result** : Both assays demonstrated a lack of mutagenic activity by behenyl alcohol. No significant and reproducible increases in the number of revertants were found in any strain and behenyl alcohol treatment group combination relative to the solvent control. In addition, no concentration-dependent enhancement of the revertant number occurred, and no differences were observed between behenyl alcohol treatments with or without metabolic activation.

**Test substance** : Behenyl alcohol (C-22 straight-chain alcohol) 1-Docosanol CASRN: 661-19-8  
Purity 98%  
source: Condea, Germany.

**Reliability** : (2) valid with restrictions  
Published reports assigned a 2

21.12.2003 (17)

**Type** : Chromosomal aberration test  
**System of testing** : Chinese Hamster V79 cells  
**Test concentration** : without act: 0, 0.6, 10 or 20 mg/L; with act 0, 1.4, 10 or 20 mg/L  
**Cytotoxic concentr.** : > 20 mg/L  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS

**Method** : The ability of behenyl alcohol to induce structural chromosome aberrations in Chinese hamster V79 cells was evaluated in vitro, with and without metabolic activation.

Behenyl alcohol was dissolved in ethanol. V79 cells were exposed to behenyl alcohol, both with and without metabolic activation. The liver microsomal fractions were obtained from 8- to 12-week-old male Wistar rats. Duplicate cultures were used. Preparations of chromosomes were completed 7, 18, and 24 hours after behenyl alcohol treatment started.

Cultures prepared at 7 and 24 hours were treated with 20 ug/ml behenyl alcohol, while cultures prepared at 18 hours were treated with 0.6, 10.0, and 20.0 ug/ml behenyl alcohol. Assays were initiated by seeding approximately 50000 to 100000 cells per dish in minimal essential medium (MEM). After 48 h (for cells harvested at 7 and 24 hours) and 55 hours (for cells harvested at 18 hours), the medium was replaced with serum-free medium containing behenyl alcohol at the appropriate dose, with and without metabolic activation.

All cultures were exposed to behenyl alcohol for four hours. Following the treatment interval, the medium was replaced with normal medium after rinsing twice with saline. Colcemia (0.2 ug/ml), a metaphase-arresting substance, was added to the cultures for the last two hours of incubation for cells harvested at 7 hours or for the last 2.5 hours of incubation for cells harvested at 18 and 28 hours. The cells were then treated on the slides in the chambers with a hypotonic solution for 20 min at 37 deg C. After incubation, the cells were fixed, stained with Giemsa, and examined microscopically. One hundred metaphases were scored for cytogenic damage per slide.

The concentrations used in this study were based on the results from a earlier range-finding study, which used the plating efficiency assay as an indicator for toxicity response. Positive controls consisted of EMS (without metabolic activation) and cyclophosphamide (with metabolic activation).

For the test substance to be scored positive, either a significant dose-related increase in the number of structural chromosomal aberrations or a significant positive response at one of the test points was required.

Statistical analysis included use of the chi-squared test, which was only performed for cells carrying aberrationsexclusive gaps. Both biological and statistical significance was considered in the assessment. Test substance significance was established where  $P < 0.05$ .

<b>Result</b>	:	Treatment with the highest concentration of 20 ug/ml behenyl alcohol did not reduce the plating efficiency of the V79 cells nor the mitotic index; however, data from the range finding study indicate that higher doses would have been toxic to cells. No relevant increases in the number of cells with structural aberrations were observed after treatment with behenyl alcohol at any concentration or time interval were observed. Positive and negative controls gave the expected results, demonstrating sensitivity of the test system.
<b>Test substance</b>	:	Behenyl alcohol (C-22 straight-chain alcohol) 1-Docosanol CASRN: 661-19-8 Purity 98% source: Condea, Germany.
<b>Conclusion</b>	:	Behenyl alcohol did not produce chromosome aberrations in V79 cells under these conditions using the highest practical non-cytotoxic concentration.
<b>Reliability</b>	:	(2) valid with restrictions Published reports assigned a 2

21.12.2003

(17)

**Type** : HGPRT assay  
**System of testing** : Chinese Hamster V79 cells  
**Test concentration** : 2.0, 7.5, 15.0, and 20.0 mg/ml  
**Cytotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : no data  
**Test substance** : other TS

**Method**

:

The potential for behenyl alcohol to induce gene mutations, in vitro, at the HGPRT locus was evaluated in Chinese hamster V79 cells, with and without metabolic activation.

Behenyl alcohol was dissolved in ethanol and V79 cells were exposed to behenyl alcohol concentrations of 2.0, 7.5, 15.0, and 20.0 mg/ml for 4 h and monitored for the loss of functional HGPRT enzyme. The final concentration of ethanol in the culture medium did not exceed 1% v/v. The selection of doses was based on the results of a previously conducted rangefinding experiment. Each concentration was tested with and without metabolic activation and the cells were subcultured twice per week. The assay was performed in two independent experiments, using identical procedures, both with and without metabolic activation. Concurrent negative and solvent controls were included, and positive controls consisted of ethylmethanesulfonate (EMS) (Merk-Schuchardt) and 7,12-dimethylbenz(a)anthracene (DMBA) (Sigma). All incubations were conducted at 37°C in a humidified atmosphere with 4.5% CO<sub>2</sub>. Methylene blue (10%) was used for staining in 0.01% KOH solution. Stained colonies with more than 50 cells were counted with a preparation microscope.

Mutant frequency was determined by seeding known numbers of cells in medium containing thioguanine to detect mutant cells, and in medium without thioguanine to determine the total number of surviving cells. For the test substance to be considered positive, a significant dose-related increase in the mutant frequency or a reproducible and significant positive response for at least one of the test points was required. The test substance also was considered to be mutagenic if there was a reproducible concentration-related increase in the mutation frequency. Such evaluation may be considered independently of an enhancement factor for induced mutants; however, this is dependent on the level of the corresponding negative control data.

**Result**

:

Gene mutation assay in Chinese hamster V79 cells. No relevant increases in mutant colony numbers were found in both independent experiments at any concentration of behenyl alcohol tested, with or without metabolic activation

**Test substance**

:

Behenyl alcohol (C-22 straight-chain alcohol) 1-Docosanol CASRN: 661-19-8  
 Purity 98%  
 source: Condea, Germany.

**Reliability**

:

(2) valid with restrictions  
 Published reports assigned a 2

21.12.2003

(17)

## 5. Toxicity

Id 68526-82-9

Date 30.12.2003

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<b>Type</b>	:	other: Salmonella typhimurium and E coli reverse mutation test
<b>System of testing</b>	:	
<b>Test concentration</b>	:	
<b>Cycotoxic concentr.</b>	:	
<b>Metabolic activation</b>	:	
<b>Result</b>	:	negative
<b>Method</b>	:	other: OECD 471 and 472
<b>Year</b>	:	
<b>GLP</b>	:	yes
<b>Test substance</b>	:	other TS
<b>Method</b>	:	Salmonella typhimurium strains: TA 1535, TA 1537, TA 98, TA 100; Escherichia coli strain: WP2uvrA-  Plate incorporation test  Metabolic activation system: Liver fraction (S9) from rats pretreated with Aroclor 1254  0, 15, 50, 150, 500, 1 500 and 5 000 µg/plate.  Each concentration was tested in triplicate with or without metabolic activation, in two independent experiments; appropriate strain specific positive control reference substances were used
<b>Result</b>	:	Precipitate noted at and above 1500 µg/plate; No cytotoxicity was observed. There were no significant increases in revertant colony numbers at any concentration, in the presence or absence of metabolic activation. Concurrent positive controls used in the test induced marked increases in the frequency of revertant colonies and the activity of the S9 fraction was found to be satisfactory
<b>Test substance</b>	:	C20-C24 alkenes, branched and linear
<b>Conclusion</b>	:	C20-C24 alkenes, branched and linear were not considered mutagenic in the bacterial strains tested
<b>Reliability</b>	:	(2) valid with restrictions  Modern guideline study under glp. Downgraded to a 2 as laboratory report was not available for review.
<b>Flag</b>	:	Critical study for SIDS endpoint
21.12.2003		(7)
<b>Type</b>	:	Chromosomal aberration test
<b>System of testing</b>	:	Human Peripheral Lymphocytes
<b>Test concentration</b>	:	
<b>Cycotoxic concentr.</b>	:	
<b>Metabolic activation</b>	:	with and without
<b>Result</b>	:	
<b>Method</b>	:	OECD Guide-line 473
<b>Year</b>	:	
<b>GLP</b>	:	no data
<b>Test substance</b>	:	other TS

<b>Method</b>	: Each concentration was tested in duplicate with or without metabolic activation (S9), in two independent experiments  Experiment 1 (repeat . see comment below): without S9, 0*, 78.13, 156.25, 312.5*, 625*, 1 250* ,2 500* 5 000* µg/mL; treatment/harvest time = 4/20 hours; positive control: ethyl methanesulphonate 750µg/mL;  with S9, 0*, 39.06, 78.13, 156.25, 312.5*, 625*, 1 250*, 2 500* 5 000* µg/mL, treatment/harvest time = 4/20 hours, positive control: cyclophosphamide 25µg/mL;  Experiment 2: without S9, 0*, 39.06, 78.13, 156.25, 312.5*, 625* 1 250*, 2 500* 5 000* µg/mL; treatment/harvest time = 20/20 hours; positive control: ethyl methanesulphonate 500µg/mL;  with S9 (increased to a final concentration of 2%), 0*, 39.06 , 78.13, 156.25, 312.5*, 625* 1 250*, 2 500* 5 000* µg/mL; treatment/harvest time: 4/20 hours, positive control: cyclophosphamide 25 µg/mL;
<b>Result</b>	: asterisk* indicates cultures selected for metaphase analysis  An initial experiment revealed: doses of 2500 or 5000 g/mL were probably beyond the maximum practical dose; an aberrant cell at the highest dose contained multiple aberrations; and weak responses in the positive control. The experiment was repeated. In the repeated Experiment 1 and Experiment 2, an oily layer was observed at and above 156.25 µg/mL and 312.5µg/mL in the presence and absence of metabolic activation, respectively.  No toxicity was observed at any concentration. The test substance did not cause any significant increases in the incidence of cells with chromosomal aberrations, polyploidy or endoreplication, at the concentrations analysed in the presence or absence of metabolic activation. Positive controls used in the test caused significant increases in the incidence of aberrant cells and the activity of the S9 fraction was found to be satisfactory.
<b>Test substance</b>	: C20-C24 alkenes, branched and linear
<b>Conclusion Reliability</b>	: C20-C24 alkenes, branched and linear was not considered to : (2) valid with restrictions
<b>Flag</b>	: Modern guideline study under glp. Downgraded to a 2 as laboratory report was not available for review. : Critical study for SIDS endpoint

21.12.2003

(19)

**Type** : other: multiple tests  
**System of testing** : Other: multiple  
**Test concentration** :  
**Cycotoxic concentr.** :  
**Metabolic activation** :  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS

**Method**

The following data are taken from the HEDSET data sheet for 1-octadecene. The full study reports were not provided in the submission.

The HEDSET documents indicate these tests were not conducted in accordance with GLP or OECD or EC testing guidelines.

**Result**

1-Octadecene was considered not mutagenic or clastogenic in the following test systems:

TEST	COMMENT	RESULT
Bacterial Rev. Muta Assay	S. typhimurium TA98, TA100, TA 1535, TA1537, TA1538. E.coli WP2, WP2uvrA. 0.2 to 2 000 mg/plate; with/without metabolic activation.	Negative
Mitotic Recombin.n	S.cerevisiae JD1. 0.01 to 5.0 mg/mL With/without metabolic activation	Negative
Chromosome Aberration	Rat liver RL1 cells. 0 to 500 µg/mL as acetone solution With/without metabolic activation.	Negative

**Test substance**

1-Octadecene RN: 112-88-9

**Reliability**

(2) valid with restrictions

Original reports not available. HEDSET documents considered reliable

21.12.2003

(20)

**Type** : other: Cell Transformation  
**System of testing** : BALB/3T3 Cells  
**Test concentration** : 0, 10, 20, 30 or 1500 µg/mL  
**Cycotoxic concentr.** : Cytotoxicity was evident at 20 µg/mL and above  
**Metabolic activation** :  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** :  
**Test substance** : other TS

<b>Method</b>	:	Mouse embryo cells BALB/3T3-A31-1-1 were treated with 0, 10, 20, 30, 1500 µg/mL of test substance in duplicate.
		Positive Control: 3-methylcholanthrene 1 µg/mL;
		Cultures were exposed to test substance for two days.
<b>Result</b>	:	Cytotoxicity was evident at 20 µg/mL and above leaving only one viable dose level, 10 g/ml.
		The number and type of transformed foci at any test substance concentration was not increased above the negative control.
		The positive control gave the expected response for transformation.
<b>Test substance</b>	:	Tetradecene (Gulftene C12-C16)
<b>Conclusion</b>	:	Tetradecene (Gulftene C12-16) did not cause cell transformation under these conditions.
<b>Reliability</b> 21.12.2003	:	(2) valid with restrictions (8) (8)
<b>Type</b>	:	Unscheduled DNA synthesis
<b>System of testing</b>	:	Primary hepatocytes from Fischer 344 rats
<b>Test concentration</b>	:	0, 100, 1000, 2000 or 4000 µg/ml
<b>Cycotoxic concentr.</b>	:	256 µg/ml in range finder
<b>Metabolic activation</b>	:	
<b>Result</b>	:	negative
<b>Method</b>	:	OECD Guide-line 482
<b>Year</b>	:	
<b>GLP</b>	:	no data
<b>Test substance</b>	:	other TS
<b>Method</b>	:	concentrations of 0, 100, 1000, 2000 or 4000 µg/mL of test substance was tested in triplicate.
		Positive Control: 2-acetylaminofluorene 0.2 µg/mL.
		Cultures were exposed to test substance and 1 mCi/mL 3H-thymidine for 18 hours.
<b>Result</b>	:	In the range finding study, cytotoxicity was reported at and above 256 µg/mL. Toxicity data were not available for the main test.
		The test substance at any concentration did not elicit an increased mean net nuclear grain count above the concurrent negative control.
		The positive control gave the expected response for UDS.
<b>Test substance</b>	:	Tetradecene (Gulftene C12-C16)
<b>Conclusion</b>	:	Tetradecene (Gulftene 12-16) did not produce an increase in unscheduled DNA synthesis under these conditions.
<b>Reliability</b>	:	(2) valid with restrictions

21.12.2003	<p>Modern guideline study. Downgraded to a 2 as laboratory report was not available for review.</p>	(16)
<p><b>Type</b> <b>System of testing</b> <b>Test concentration</b> <b>Cycotoxic concentr.</b> <b>Metabolic activation</b> <b>Result</b> <b>Method</b> <b>Year</b> <b>GLP</b> <b>Test substance</b></p>	<p>: HGPRT assay : CHO Cells : 0, 4, 16, 128, 512, 1024 or 2048 µg/mL : 1024 : with and without : negative : OECD Guide-line 476 : : no data : other TS</p>	
<b>Method</b>	<p>: Cells: Chinese Hamster Ovary (CHO)</p> <p>Metabolic activation system: Liver fraction (S9) from rats pretreated with Aroclor 1254</p> <p>Dosing schedule: 0, 4, 16, 128, 512, 1024 or 2048 µg/mL each concentration was tested in triplicate with or without metabolic activation (S9)</p> <p>Positive controls: Without S9: ethyl methanesulphonate 100µg/mL; With S9: benzo[a]pyrene 4 µg/mL;</p>	
<b>Result</b>	<p>: Exposure period was 5 hours</p> <p>: Toxicity was observed at 1024 and 2048 µg/mL in the presence and absence of metabolic activation.</p> <p>The test substance did not cause any significant increases in the incidence of mutant colonies in the presence or absence of metabolic activation.</p> <p>Positive controls used in the test caused marked increases in the incidence of mutant colonies and the activity of the S9 fraction was found to be satisfactory.</p>	
<b>Test substance</b>	<p>: Tetradecene (Gulftene C12-C16)</p>	
<b>Conclusion</b>	<p>: Tetradecene (Gulftene 12-16) did not induce gene mutations in CHO cells.</p>	
<b>Reliability</b>	<p>: (2) valid with restrictions</p>	
21.12.2003	<p>Modern guideline study. Downgraded to a 2 as laboratory report was not available for review.</p>	(21)

## 5.6 GENETIC TOXICITY 'IN VIVO'

<b>Type</b>	:	Micronucleus assay
<b>Species</b>	:	mouse
<b>Sex</b>	:	male
<b>Strain</b>	:	other: Crl:CD-1 (ICR) BR
<b>Route of admin.</b>	:	i.p.
<b>Exposure period</b>	:	24 and 48 hours
<b>Doses</b>	:	500, 1000 or 2000 mg/kg bw
<b>Result</b>	:	negative
<b>Method</b>	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
<b>Year</b>	:	
<b>GLP</b>	:	
<b>Test substance</b>	:	other TS
<b>Method</b>	:	<p>7 males/24 hour, vehicle and positive control, and mid, low and high dose group; 7 males/48 hour, vehicle control and high dose group; 5 males/positive control group.</p> <p>administration:  Test substance: 500 mg/kg (low)  1000 mg/kg (mid)  2 000 mg/kg (high)</p> <p>Positive control: cyclophosphamide 50 mg/kg;  Vehicle control: arachis oil;  TS administered via intraperitoneal injection at a constant volume of 10 mL/kg bw. Positive control was administered orally.</p> <p>Sacrifice:  Vehicle and positive control, low, mid and high dose animals were sacrificed 24 hours after dosing.  Remaining animals of the vehicle control group and high dose animals were sacrificed 48 hours after dosing.</p>
<b>Result</b>	:	<p>Clinical observations:  No mortality.  No clinical signs of toxicity.</p> <p>Micronuclei score:  No significant increase in micronucleated PCE due to treatment with test substance at either sampling time. No statistically significant decrease in the PCE/NCE ratio at 24 or 48 hours.  The positive control caused a significant increase in micronucleated PCE.</p>
<b>Test substance</b>	:	C20-C24 Alkenes, branched and linear
<b>Conclusion</b>	:	C20-C24 alkenes, branched and linear did not induce a significant increase in micronucleated PCE in bone marrow cells of the mouse in vivo.
<b>Reliability</b>	:	(2) valid with restrictions
		Modern guideline study under glp. Downgraded to a 2 as laboratory report was not available for review.

17.12.2003

(26)

**Type** : Micronucleus assay  
**Species** : mouse  
**Sex** : male/female  
**Strain** : NMRI  
**Route of admin.** : gavage  
**Exposure period** : 24, 48 or 72 hours  
**Doses** : 0, 50, 150, or 500 mg/kg-bw  
**Result** : negative  
**Method** :  
**Year** :  
**GLP** : yes  
**Test substance** : other TS:

**Method**

:

The potential for behenyl alcohol to induce micronuclei in polychromatic erythrocytes (PCE) in bone marrow of NMRI mice was evaluated in vivo. Animals at least 10 weeks old (BRL Tierfarm Füllinsdorf, Switzerland) were individually housed in Markrolon Type 1 cages with wire mesh tops and granulated soft wood bedding. Animals were housed in a room designed to maintain adequate environmental conditions (21°C, 12-h photocycle; relative humidity was not regulated). Animals were fed both a standard pellet diet and tap water, ad libitum, during the study.

Prior to treatment with behenyl alcohol, mice were fasted for 18 h, but continued to receive water ad libitum. Twelve mice (6 males and 6 females) were administered a single oral dose of 0, 50, 150, or 500 mg behenyl alcohol/kg body weight suspended in polyethylene glycol. Doses were based on the results from a previously conducted experiment in which 500 mg/kg body weight was estimated to be the maximum attainable dose. The volume administered was 10 ml/kg body weight. Cyclophosphamide (CPA) was used as the positive control at 40 mg/kg body weight.

At 24, 48, or 72 h after dosing, animals were killed and bone marrow cells were collected for micronuclei analysis. Only 5 mice/sex/dose group were evaluated in the event that remaining animals of each treatment group died spontaneously, or due to gavage error. Animals were killed by cervical dislocation. The femora were removed, the epiphyses were cut off, and the marrow was flushed out with fetal calf serum. The cell suspension was centrifuged at 1500 rpm for 5 min and the supernatant was discarded. A small drop of resuspended cell pellet was spread on a slide. The smear was air-dried, stained and coverslips were mounted. At least 1 slide per sample was made and scored for micronuclei and polychromatic-normochromatic (NCE) cell ratio. For each animal, 1000 PCEs were scored for micronuclei.

For the test substance to be classified as mutagenic, either a statistically significant dose-related increase in the number of micronucleated polychromatic erythrocytes or a reproducible statistically significant positive response for at least one of the test points was required.

Statistical analysis was conducted using the Mann-Whitney test; however, both biological significance and statistical significance were considered in the study. Significance was established where  $P < 0.05$ .

**Result**

:

As shown below in the Table, there was no increase in the percentage micronucleated PCE, or in the PCE:NCE ratio of mice at any preparation interval after treatment with any dose level.

Treatment	Dose (mg/kg)	Harvest time (h)	percent micro nucleated (mean)	Ratio PCE:NCE (mean)
Vehicle control	0	24	0.03	1.27
		48	0.09	1.05
		72	0.09	1.41
CP (positive)	40	24	0.71	0.93
Behenyl alcohol	50	24	0.07	0.98
		48	0.10	1.06
		72	0.09	1.33
	150	24	0.08	1.07
		48	0.04	1.01
		72	0.05	1.55
500	24	0.07	1.11	
	49	0.05	1.23	
	72	0.07	1.46	

**Test substance** : Behenyl alcohol (C-22 straight-chain alcohol) 1-Docosanol CASRN: 661-19-8  
Purity 98%  
source: Condea, Germany.

**Conclusion** : Test material did not induce micronuclei in the bone marrow of mice under these conditions.

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

Guideline-like GLP study. Dosing rationale not provided. Published study assigned 2.

21.12.2003

(17)

### 5.8.1 TOXICITY TO FERTILITY

**Type** : One generation study

**Species** : rat

**Sex** : male/female

**Strain** : other: Crl:CD BR VAF/Plus

**Route of admin.** : gavage

**Exposure period** :

**Frequency of treatm.** :

**Premating exposure period**

**Male** : 28 days

**Female** : 14 days

**Duration of test** :

**No. of generation studies** : 1

**Doses** : 100, 500, 1000 mg/kg

**Control group** : yes, concurrent vehicle

**NOAEL parental** : <= 100 mg/kg bw

**NOAEL F1 offspring** : = 1000 mg/kg bw

**Method** :

Number/sex of animals: 12 males/group 20 females/group (12 females assigned to breeding phase and 8 females assigned as satellite females)

Method of administration: Oral (gavage)

Doses: 0, 100, 500 or 1000 mg/kg/day (dose volume 5mL/kg) for a minimum of 42 days;

Vehicle: corn oil.

Dosing Schedule: Males:

Day 0 to 28 - Pretreatment;

Day 29 to 42 - Mating;

Day 43 to 47 - Dosing after mating.

Satellite females:

Day 0 to 49 . Dosing period.

Breeding females:

Day 0 to 14 . Pretreatment;

Day 15 to 42 . Dosing during mating and lactation;

Day 43 to 51 - Dosing during lactation and until termination

Terminal kill schedule Day 43. euthanasia of unselected males (4 rats/sex/group).

Days 45 to 47. neurotoxicity and clinical pathology evaluations (8 rats/sex/group), histopathology (5 rats/sex/group).

Days 42 to 51 . euthanasia and necropsy of breeding females (F0)and F1 pups.

Test methods: OECD TG 422 (modified)

### Result

:

MORTALITY:

F0 males and satellite females: Nil.

F0 females: In the 500 mg/kg/day group, one female with evidence of mating failed to deliver and was euthanised on post breeding day 25 and one female was euthanised with total litter loss on Day 43.

CLINICAL OBSERVATIONS:

F0 males, satellite females and F0 females:

Urine stain and salivation noted in the 500 and 1000 mg/kg/day groups. No other consistent observations.

Functional Observation Battery (FOB) and Motor Activity:

F0 males and satellite females:

No compound related differences in the FOB and motor activity tests between control and treated groups.

CLINICAL PATHOLOGY:

F0 males and satellite females:

Serum Chemistry:

Significantly increased alanine transferase (ALT) activity in males. In females, significantly decreased sodium values at all treatment doses and significantly increased cholesterol in the 500 and 1000 mg/kg/day groups.

HEMATOLOGY:

Slight decreases in mean erythrocyte count and haematocrit at all treatment doses and in haemoglobin and mean cell volume at 1000 mg/kg/day in rats of each sex. These changes were only significant in females.

Significantly increased mean cell haemoglobin concentration in females of the 100 and 1000 mg/kg/day group and in males of the 1000 mg/kg/day group.

**PATHOLOGY:**

F0 males and satellite females:

Organ Weights:

Significantly increased absolute liver weight and liver weight relative to brain weight in animals of the 500 and 1 000 mg/kg/day group.

Significant findings in females only were decreased spleen weight (relative to brain weights) in the 1000 mg/kg/day group and increased kidney weight in the 500 mg/kg/day group.

Macroscopic:

In males, pitted kidneys were observed in the 500 and 1000 mg/kg/day groups.

Microscopic:

Treatment related effects were observed in kidneys of all test males (dose-related increased eosinophilic hyaline droplets in the proximal convoluted tubules, a finding commonly associated with hydrocarbon nephropathy).

Minimal to moderate hepatocellular vacuolation was observed in animals of the 500 and 1000 mg/kg/day groups.

F0 females:

Macroscopic:

No test related findings were observed. The animal euthanized on post breeding Day 25 was found to be non gravid. The animal euthanized on Day 43 was found to have implantation sites.

**FERTILITY, GESTATION, PARTURITION AND LACTATION:**

Mating and fertility indices, precoital intervals and gestation length were comparable among the groups.

**F1 GENERATION FINDINGS:**

No treatment related developmental effects through to lactation Day 4.

**Test substance**

:

**Conclusion**

:

1-Tetradecene CASNO 1120-36-1 (the substance used was blended from three different suppliers of 1-tetradecene)

**Reliability**

:

Based upon liver weight increase and hepatocyte cytoplasmic vacuolation observed at 500 and 1000 mg/kg/day, the NOAEL for systemic toxicity in satellite females was 100 mg/kg/day. No NOAEL for systemic toxicity was established for males because of hydrocarbon nephropathy noted at all dose levels. The NOAEL for reproductive, developmental or neurotoxicity was 1000 mg/kg/day in rats of each sex.

**Flag**

21.12.2003

:

(1) valid without restriction  
Modified guideline study downgraded to 2 because original laboratory report was not available for review.

Critical study for SIDS endpoint

(10)

**Type**

:

One generation study

**Species**

:

rat

**Sex**

:

male/female

## 5. Toxicity

Id 68526-82-9

Date 30.12.2003

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**Strain** : Sprague-Dawley  
**Route of admin.** : gavage  
**Exposure period** :  
**Frequency of treatm.** : daily  
**Premating exposure period**  
    **Male** : 71 days  
    **Female** : 14 days  
**Duration of test** :  
**No. of generation** :  
**studies**  
**Doses** : 10, 100, 1000 mg/kg  
**Control group** : yes, concurrent vehicle  
**NOAEL F1 offspring** : = 1000 ml/kg bw  
**NOAEL F2 offspring** : = 1000 ml/kg bw  
**Result** : No reproductive or developmental effects  
**Method** : other: ICH Harmonized Tripartite Repro Effectx Medicinal Prod  
**Year** :  
**GLP** : yes  
**Test substance** : other TS: surrogate

**Method** :

Adult Sprague-Dawley (Charles River, Margate, Kent, England) rats of each sex were obtained at approximately 5 to 6 weeks of age. Rats were acclimated to the laboratory environment for 6 days prior to the initiation of dosing. During the acclimation period, rats were observed daily. Male rats weighed between 193 and 240 g and were 6 to 7 weeks of age at study start. Female rats were obtained eight weeks after the males. Female rats weighed between 208 and 262 g and were 10 to 11 weeks of age at study start. During the acclimation and pre-mating periods, 10 rats (5 males and 5 females) were housed per stainless-steel cage. During the mating period, 1 male and 1 female were housed in a polypropylene cage with stainless-steel mesh lids and floors. Five females were housed together during the gestation period, while 5 males were housed together after the mating period was complete. Cages were equipped with polyethylene or polycarbonate bottles and sipper tubes and were placed in rooms designed to maintain adequate environmental conditions (18°C; 55% relative humidity, 12-h photocycle).

Feed was an expanded rodent diet containing no added antibiotic, or other chemotherapeutic or prophylactic agent. Water was local tapwater. Both food and water were available to the rats ad libitum.

**DOSAGE LEVELS.** Eighty-eight CD male rats and eight-eight CD female rats were administered the test substance formulated to supply targeted dosages of 0, 10, 100, or 1000 mg behenyl alcohol/kg body weight/day (Groups 1, 2, 3, and 4, respectively). Each treatment group consisted of 44 rats (22 males and 22 females). Animals were dosed by gavage at 5 ml/kg body weight. The volume given to each animal was calculated from body weights measured immediately before each administration. Males were treated with behenyl alcohol daily for 71 days prior to mating, during mating, and until termination. Females were treated with the test substance for 15 days prior to mating, during mating, and up to Day 17 of gestation.

Dosing Solutions were prepared by weighing the required amount of behenyl alcohol into a glass container and heating the container to

approximately 80°C until the behenyl alcohol was molten. Vehicle (1% Tween 80) was heated in a water bath to at least 75°C and combined with the molten behenyl alcohol under continuous magnetic stirring, to a concentration of 20% behenyl alcohol. The resulting suspension was slowly cooled, with homogenization to a temperature below 60°C, and then further cooled in a water bath to a temperature of 30°C. Once the resulting suspension reached this temperature, it was again slowly homogenized for at least 2 min and allowed to cool to room temperature. The concentrated suspension was further diluted to achieve the proper dosage levels.

**IN-LIFE DATA:** Rats were observed daily at cage side for evidence of reaction and general health. A thorough macroscopic examination of the visceral organs was completed on any animal that died during the study. Prior to mating, food and water consumption for males and females was recorded weekly and daily, respectively. During the gestation period, food and water consumption was measured only for females during the following time periods: Gestation Days 0 to 2, 3 to 6, 7 to 9, 10 to 13, 14 to 17, and 18 to 19, inclusive. Male and female body weight gains were measured twice weekly until mating. Following mating, male body weight gains were measured twice weekly for the remainder of the study, and body weight gains for females were recorded on GD 0, 3, 7, 10, 14, 18, and 20. In addition, starting 10 days before the mating period, vaginal smear samples were obtained daily from all females to assess the regularity and duration of estrous cycles.

**REPRODUCTIVE PERFORMANCE:** Trays beneath the cages were checked for ejected copulation plugs every morning during the mating procedure. Vaginal smears from each female were also examined for the presence of spermatozoa. The length of the mating period was recorded (time elapsing between initial pairing and detection of mating) and Gestation Day 0 was designated as the day in which evidence of mating was found.

**REPRODUCTIVE ENDPOINTS.** Females were killed on Day 20 of gestation using carbon dioxide, and uterine contents were examined. Each female was macroscopically examined for evidence of disease or adverse reaction to test substance. Corpora lutea in each ovary were counted. The reproductive tract, including the ovaries, was then dissected out. For each female, the numbers of pre- and post-implantation sites, early and late resorption sites, and viable fetuses, as well as the distribution of fetuses in each uterine horn, were examined. The uterus of any female that was not gravid was stained with ammonium sulfide solution and examined for implantation sites.

Each fetus was weighed, given a detailed external examination, and uniquely identified within the litter with respect to the uterine position. Placenta were weighted and examined macroscopically for any abnormalities. The neck, thoracic, and abdominal cavities were removed from half of the fetuses, the contents of the thoracic and abdominal cavities were examined, and the sex was recorded. These fetuses were eviscerated, fixed in methylated spirit, processed and stained with Alizarin Red, and subjected to a skeletal examination. The remaining fetuses were placed in Bouin's fixative and internally examined using a modification of the Wilson free-hand serial sectioning technique.

Following necropsy of the females, males were killed with carbon dioxide, and examined externally and internally. Reproductive organ weights were

recorded. The left vas deferens was ligated to obtain a 5-microliter sample from the cauda epididymis. The sample was diluted in medium and mixed to assess for motility. The number of spermatozoa was assessed using a hemocytometer after further diluting the sample with 4% v/v neutral buffered formaldehyde.

STATISTICS: : To test the statistical significance of suggestive intergroup differences, one-way analysis of variance and t test were performed on body weights, body weight changes, and food and water consumption. Organ weights were evaluated by Dunnett's or Behren's-Fisher's tests. Nested analysis of variance and weighed t test were conducted on fetal and placental weights. Differences with an associated probability of  $P < 0.05$  were considered statistically significant.

**Remark** : Result is supported by a rabbit reproduction study reported in the same publication.

**Result** : All female rats survived to scheduled sacrifice. One male treated with 1000 mg/kg demonstrating severe adverse clinical signs and a decrease in body weight was killed during week 6. This was the only death that occurred in the study and it was not considered treatment related. No other remarkable clinical observations were seen in any of the treated animals. Body weight gains, food and water consumption for rats of each sex of all dose groups, were comparable to controls throughout the study. No compound-related differences in female estrous cycles or mating performance and fertility were observed in any of the treatment groups when compared to the control group. Macroscopic findings at terminal necropsy revealed no findings attributable to test substance. No differences were observed in the number of corpora lutea, pre- and postimplantation sites, early and late resorptions, and viable fetuses. Fetal and placental weights were not affected by treatment with behenyl alcohol. Fetal sex ratios were comparable between all treatment groups and controls.

Parameter	DOSE (mg/kg-day)			
	0	10	100	1000
Number pregnant	22	22	22	21
Corpora lutea	17.8	18.4	18.7	18.9
Implantations	17.2	17	18.1	18
Viable young				
Male	8.4	8.4	8.5	8.6
Female	8	7.5	8.5	8.3
Total	16.4	15.9	17	16.9
Resorptions				
Early	0.82	1.09	1.14	1.05
Late	0	0	0	0
Total	0.82	1.09	1.14	1.05
Implantation loss (%)				
Pre	3.3	8.3	3.2	5.8
Post	4.7	6.4	6.3	5.8

Macroscopic, internal, and skeletal examinations of the fetuses, revealed no variations that were not comparable to historical control values. There were no observed effects related to behenyl alcohol treatment in this study. No significant macroscopic findings were reported in males treated with

		behenyl alcohol. Absolute and relative body weights of reproductive organs were similar between the treatment groups and the control group. Evaluation of sperm number and motility revealed no findings attributable to behenyl alcohol treatment.
<b>Test substance</b>	:	Behenyl alcohol (C-22 straight-chain alcohol) 1-Docosanol CASRN: 661-19-8 Purity 98% source: Condea, Germany.
<b>Conclusion</b>	:	There were no observed effects related to behenyl alcohol treatment in this reproduction study.
<b>Reliability</b>	:	(1) valid without restriction
		Modern guideline study under GLPs
21.12.2003		(18)

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

<b>Species</b>	:	rat
<b>Sex</b>	:	female
<b>Strain</b>	:	Wistar
<b>Route of admin.</b>	:	gavage
<b>Exposure period</b>	:	Days 6 to 15 of gestation
<b>Frequency of treatm.</b>	:	Daily
<b>Duration of test</b>	:	
<b>Doses</b>	:	0, 144, 720 or 1440 mg/kg-day
<b>Control group</b>	:	yes, concurrent vehicle
<b>NOAEL maternal tox.</b>	:	= 1440 mg/kg bw
<b>NOAEL teratogen.</b>	:	= 1440 mg/kg bw
<b>Method</b>	:	OECD Guide-line 414 "Teratogenicity"
<b>Year</b>	:	
<b>GLP</b>	:	yes
<b>Test substance</b>	:	
<b>Method</b>	:	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. \Test material was administered at doses of 144, 720, or 1440 mg/kg/day. A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
<b>Remark</b>	:	Statistical methods: Dunnett's test, Fisher's exact test
<b>Test substance</b>	:	Alcohols, C7-11-branched and linear, CASNO 85566-14-9
<b>Conclusion</b>	:	The test material consisted of linear alcohols and alpha-methyl branched alcohols ranging in carbon chain length from C7 to C11 C7-11 Alcohol does not produce signs of toxicity in the dam or the fetus at these dose levels. C7-11 Alcohol is not embryo or fetotoxic under the conditions of this study.
<b>Reliability</b>	:	(2) valid with restrictions Reliable with restrictions - Only 10 animals per group, instead of the recommended 20 (OECD 414), were employed
13.11.2002		(27) (28)

**Species** : rat  
**Sex** : male/female  
**Strain** : other: Crl:CD BR VAF/Plus  
**Route of admin.** : gavage  
**Exposure period** : Premating through gestation  
**Frequency of treatm.** : daily  
**Duration of test** :  
**Doses** : 100, 500, 1000 mg/kg  
**Control group** : yes, concurrent vehicle  
**NOAEL maternal tox.** : = 100 mg/kg bw  
**NOAEL teratogen.** : = 1000 mg/kg bw  
**Result** : negative  
**Method** : other: OECD 422 (modified)  
**Year** :  
**GLP** : yes  
**Test substance** : other TS

**Method**

:  
 Number/sex of animals: 12 males/group 20 females/group (12 females assigned to breeding phase and 8 females assigned as satellite females)

Method of administration: Oral (gavage)

Doses: 0, 100, 500 or 1000 mg/kg/day (dose volume 5mL/kg) for a minimum of 42 days;

Vehicle: corn oil.

Dosing Schedule: Males:

Day 0 to 28 - Pretreatment;

Day 29 to 42 - Mating;

Day 43 to 47 - Dosing after mating.

Satellite females:

Day 0 to 49. Dosing period.

Breeding females:

Day 0 to 14. Pretreatment;

Day 15 to 42. Dosing during mating and lactation;

Day 43 to 51. Dosing during lactation and until termination.

Terminal kill schedule Day 43. Sacrifice of unselected males (4 rats/sex/group).

Days 45 to 47. Neurotoxicity and clinical pathology evaluations (8 rats/sex/group), histopathology (5 rats/sex/group).

Days 42 to 51. Sacrifice and necropsy of breeding females (F0) and F1 pups.

**Result**

:  
 Mortality:

F0 males and satellite females: None

F0 females: In the 500 mg/kg/day group, one female with evidence of mating failed to deliver and was sacrificed on post breeding day 25 and one female was sacrificed with total litter loss on Day 43.

### Clinical observations:

F0 males, satellite females and F0 females:

Urine stain and salivation was noted in the 500 and 1000 mg/kg/day groups. Other observations were noted sporadically.

### Functional Observation Battery (FOB) and Motor Activity:

F0 males and satellite females:

No test-substance related differences in the FOB and motor activity tests between the control and treated groups.

### Clinical Pathology:

F0 males and satellite females:

Serum Chemistry:

Significantly increased alanine transferase (ALT) activity in males. In females, significantly decreased sodium values at all treatment doses and significantly increased cholesterol in the 500 and 1 000 mg/kg/day groups.

### Haematology:

Slight decreases in mean erythrocyte count and haematocrit at all treatment doses and in haemoglobin and mean cell volume at 1000 mg/kg/day in both sexes. These changes were only significant in females. Significantly increased mean cell haemoglobin concentration in females of the 100 and 1000 mg/kg/day group and in males of the 1000 mg/kg/day group.

### Pathology:

F0 males and satellite females:

Organ Weights:

Significantly increased absolute liver weight and liver weight relative to brain weight in animals of the 500 and 1 000 mg/kg/day group. Significant findings in females only were decreased spleen weight (relative to brain weights) in the 1 000 mg/kg/day group and increased kidney weight in the 500 mg/kg/day group.

### Macroscopic:

In males, pitted kidneys were observed in the 500 and 1 000 mg/kg/day groups.

### Microscopic:

Treatment related effects were observed in kidneys of all test males (dose-related increased eosinophilic hyaline droplets in the proximal convoluted tubules, a finding commonly associated with hydrocarbon nephropathy). Minimal to moderate hepatocellular vacuolation was observed in animals of the 500 and 1 000 mg/kg/day groups.

F0 females:

Macroscopic:

No test related findings were observed. The animal euthanised on post breeding Day 25 was found to be non gravid. The animal euthanised on Day 43 was found to have implantation sites.

### Fertility, Gestation, Parturition and Lactation:

Mating and fertility indices, precoital intervals and gestation length were comparable among the groups.

**Test substance** : F1 generation findings:  
No treatment related developmental effects through to lactation Day 4.  
1-Tetradecene CASNO 1120-36-1 (the substance used was blended from three different suppliers of 1-tetradecene)

**Conclusion** : Based upon liver weight increase and hepatocyte cytoplasmic vacuolation observed at 500 and 1000 mg/kg/day, the NOAEL for systemic toxicity in satellite females was 100 mg/kg/day. No NOAEL for systemic toxicity was established for males because of hydrocarbon nephropathy noted at all dose levels. The NOAEL for reproductive, developmental or neurotoxicity was 1000 mg/kg/day in rats of each sex.

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

21.12.2003 Modified guideline study downgraded to 2 because original laboratory report was not available for review

(1)

- 
- (1) Combined Repeated Dose Toxicity Study with Reproduction/Developmental Screening Test and Neurotoxicity Study in Rats using 1-tetradecene (Springborn Laboratories Inc 1995) As reported in: NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME, FULL PUBLIC REPORT, GULFTENE C14 ISOMERISED OLEFINS NA/844 26 February 2001
  - (2) A Thirteen-Week Inhalation Toxicity Study with Heavy Oxo Ends in Rats, Project No. 84-7737 (BD-84-359). BioDynamics Inc, sponsored by Monsanto Company, report dated 16 January 1987.
  - (3) Acute Toxicity of Heavy Oxo Ends to Bluegill Sunfish. Static Assay Report #29998 Analytical Bio-Chemistry Laboratories Inc, Submitted to Monsanto Chemical Co. January 28, 1983
  - (4) Acute Toxicity of Heavy Oxo Ends to Rainbow Trout. Static Assay Report #29999 Analytical Bio-Chemistry Laboratories Inc, Submitted to Monsanto Chemical Co. January 28, 1983
  - (5) Acute Toxicity of Heavy Oxo-Ends (HOE) to Daphnia Magna. Report Number ES-82-SS-63 of MIC Environmental Sciences, Monsanto Chemical Co, 9/10/1982
  - (6) An Acute Inhalation Study of Heavy Oxo Ends in the Rat. Final Report. Bio/dynamics Inc. Project No 84-7726 Submitted to Monsanto. August 1, 1985.
  - (7) Bacterial Reverse Mutation Test using C20-C24 alkenes, branched and linear (Safepharm Laboratories Limited 1998) As cited in The National (Australia) Industrial Chemicals Notification and Assessment Scheme Full Public Report for Gulfteen C14 Isomerized Olefins, 3 October 2000.
  - (8) BALB/3T3 Transformation Test Using Gulftene 12-16 (Gulf Life SciencesCenter 1983). As cited in The National (Australia) Industrial Chemicals Notification and Assessment Scheme Full Public Report for Gulfteen C14 Isomerized Olefins, 3 October 2000.
  - (9) Calculated by TRA using EPIWIN 3.05
  - (10) Combined Repeated Dose Toxicity Study with Reproduction/Developmental Screening Test and Neurotoxicity Study in Rats using 1-tetradecene (Springborn Laboratories Inc 1995) As reported in: NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME, FULL PUBLIC REPORT, GULFTENE C14 ISOMERISED OLEFINS NA/844 26 February 2001
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  - (12) EPIWIN 3.05, Syracuse Research Corporation, AOP Program v1.90
  - (13) Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114994A. 1997. As cited in Revised Robust Summaries for the Olefin Hydroformylation Products Category 15 October 2002.

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- (14) Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 119294A. 1997. As cited in Revised Robust Summaries for the Olefin Hydroformylation Products Category 15 October 2002.
- (15) Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 180294A. 1997. As cited in Revised Robust Summaries for the Olefin Hydroformylation Products Category 15 October 2002.
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- (20) In Vitro Genotoxicity of 1-octadecene (EU 1995) as cited in HEDSET and as cited in The National (Australia) Industrial Chemicals Notification and Assessment Scheme Full Public Report for Gulfteen C14 Isomerized Olefins, 3 October 2000.
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- (24) IUDLID-2000 document for Fatty acids C10-14 CASNO 90990-09-3, European Chemicals Bureau, 2000
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- (27) No adverse effects were observed at any dose of C7-9-11 Alcohol. This included changes in body weight and food consumption by the dams, reproductive parameters, and signs of fetal toxicity.

## 9. References

Id 68526-82-9

Date 30.12.2003

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