201-14960

IUCLID

Data Set

Robust Summaries

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Existing Chemical	:	ID: 76899-35-9
CAS Name	:	Eicosenoic acid, methyl ester
CAS No.	:	76899-35-9
Molecular Formula	:	C21H40O2
Molecular Weight	:	324.55
Status	:	
Memo	:	Eicosenoic acid, Crompton US HPV
Printing date	:	17.12.2003
Revision date	:	
Date of last update	:	17.12.2003
Number of pages	:	1
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	98.1 °C
Sublimation	:	
Method	:	other: Estimation using MPBPWIN v 1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Reliability	:	(2) valid with restrictions

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2.2 BOILING POINT

Value	:	375.8 °C at
Decomposition	:	
Method	:	other: Estimation using MPBPWIN v1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Reliability	:	(2) valid with restrictions

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2.4 VAPOUR PRESSURE

Value	:	.0000083 hPa at °C
Decomposition	:	
Method	:	other (calculated): MPBPWIN v1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Reliability	:	(2) valid with restrictions

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2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	9 at °C
pH value	:	
Method	:	other (calculated): KOWWIN v1.66
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Reliability	:	(2) valid with restrictions

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water

pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: WSKOW v1.40
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Reliability	:	(2) valid with restrictions

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3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm^3
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated): AOP v1.90
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Result	:	rate constant (cis-isomer) = 77.5E-12 cm3/molecule-sec rate constant (trans-isomer) = 85.14E-12 cm3/molecule-sec T1/2 (cis-isomer) = 1.655 hours T1/2 (trans-isomer) = 1.507 hours
Reliability	:	(2) valid with restrictions

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3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other (calculated): HYDROWIN v1.67
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9
Result	:	T1/2 (pH 8) = 266 days T1/2 (pH 7) = 7.28 years
Reliability	:	(2) valid with restrictions

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3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
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	:	other: EPIWIN Level III Fugacity Model

Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.098	1.29	1000
Water	7.3	360	1000
Soil	28	360	1000
Sediment	64.6	1440	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.34E-12	981	18.3	32.7	0.609
Water	4.84E-11	261	136	8.71	4.52
Soil	1.39E-13	1000	0	33.4	0
Sediment	1.45E-11	579	24	19.3	0.802

Persistence time: 620 hr
Reaction time: 659 hr
Advection time: 10400 hr
Percent reacted: 94.1
Percent advected: 5.94

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):
Air: 1.291
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.921 (weeks)

Advection times (hr):
Air: 100
Water: 1000
Sediment: 5E+4

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3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Contact time :
Degradation : (±) % after
Result : readily biodegradable
Deg. product :
Method : other: Calculated using BIOWIN v4.00
Year : 2003
GLP :
Test substance : Chemical name: Eicosenoic acid, methyl ester (Z)-
CAS No.: 76899-35-9

Result : MITI Linear Biodegradation Probability = 0.894

MITI Non-linear Biodegradation Probability - 0.929

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4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	other: Estimation
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	.009
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9

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4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	other: Estimation
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	.00011
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9

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4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	.0009
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2003
GLP	:	
Test substance	:	Chemical name: Eicosenoic acid, methyl ester (Z)- CAS No.: 76899-35-9

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5.1.1 ACUTE ORAL TOXICITY

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

(1) US EPA, EPIWIN v3.10, EPI Suite Software, 2000