IUCLID

Data Set

Existing Chemical	:	ID: 4767-03-7
CAS No.	:	4767-03-7
EINECS Name	:	2,2-bis(hydroxymethyl)propionic acid
EC No.	:	225-306-3
Molecular Formula	:	C5H10O4

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	15.12.2006

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	15.12.2006
Status	:	
Memo	:	GEO
Printing date	:	10.01.2007
Revision date	:	
Date of last update	:	02.01.2007
Number of pages	:	8
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
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	:	= 189 - 191 °C
Sublimation	:	
Method	:	other
Year	:	2000
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	ISHOW - Information System for Hazardous Organics in Water Details: Sample Record ISHOW, sponsored by the Office of Toxic Substances of the EPA, was developed by the EPA laboratory in Duluth, Minnesota in conjunction with the University of Minnesota. This database of 17,159 records includes physical property data on more than 5,700 different chemicals with bibliographic references to the original sources. Not all properties are recorded for all substances.
Test substance	:	Purity: 98%
Reliability	:	(2) valid with restrictions Modeled data
Flag	:	Critical study for SIDS endpoint

15.12.2006 (1)

Value	:	= 181 - 185 °C
Sublimation	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Reliability of 2 assigned because data are taken from a reliable secondary literature source

15.12.2006 (5)

Value	:	= 170 - 180 °C
Decomposition	:	yes, at = 230 °C
Sublimation	:	
Method	:	other
Year	:	1999
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	There is no known decomposition/transformation except at elevated temperatures.
Test substance	:	dimethylolpropionic acid; purity = 99.7%
Reliability	:	(2) valid with restrictions Internal company data

15.12.2006 (4)

Value	:	= 189 - 191 °C
Sublimation	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity = 98%
Reliability	:	(4) not assignable Safety data sheet

15.12.2006 (2)

2.2 BOILING POINT

Decomposition	:	
Method	:	other: technical discussion
Year	:	2006
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	DMPA is a solid; determination of the boiling point is not applicable.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.12.2006

2.4 VAPOUR PRESSURE

Value	:	1 hPa at 160 °C
Decomposition	:	
Method	:	
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(4) not assignable Safety data sheet
Flag	:	Critical study for SIDS endpoint

02.01.2007 (6)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= -.95 at °C
pH value	:	
Method	:	
Year	:	1999
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	dimethylolpropionic acid; purity = 99.7%
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

15.12.2006 (4) (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 11 mg/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	

Stable	:	
Deg. product	:	
Method	:	other
Year	:	1999
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	dimethylolpropionic acid; purity = 99.7%
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

21.12.2006 (4)

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/cm³
Rate constant	:	= .000000000009 cm³/(molecule*sec)
Degradation	:	= 50 % after 14.2 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2006
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Method :

```
AOP Program (v1.91) Results:
============================
SMILES : O=C(O)C(CO)(CO)C
CHEM  : Propanoic acid, 3-hydroxy-2-(hydroxymethyl)-2-methyl-
MOL FOR: C5 H10 O4
MOL WT : 134.13
```

Result :

```
--------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ---------
Hydrogen Abstraction      =  8.2090 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.8000 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 =  9.0090 E-12 cm3/molecule-sec
  HALF-LIFE =    1.187 Days (12-hr day; 1.5E6 OH/cm3)
  HALF-LIFE =   14.247 Hrs
-----------SUMMARY (AOP v1.91): OZONE REACTION ---------
****** NO OZONE REACTION ESTIMATION ******
 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
```

Reliability : (2) valid with restrictions
Data obtained through use of recognized model

Flag : Critical study for SIDS endpoint

18.12.2006 (3)

3.1.2 STABILITY IN WATER

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: calculated

Year : 2006

Method : Level III Fugacity Model (Full-Output):
==========
Chem Name : Propanoic acid, 3-hydroxy-2-(hydroxymethyl)-2-methyl-
Molecular Wt: 134.13
Henry's LC : 1.71e-012 atm-m3/mole (Henrywin program)
Vapor Press : 1.28e-006 mm Hg (Mpbpwin program)
Liquid VP : 5.36e-005 mm Hg (super-cooled)
Melting Pt : 189 deg C (user-entered)
Log Kow : 0.95 (user-entered)
Soil Koc : 3.65 (calc by model)

Result : Mass Amount Half-Life Emissions

	(percent)	(hr)	(kg/hr)
Air	8.86e-005	28.5	1000
Water	40.5	208	1000
Soil	59.5	208	1000
Sediment	0.0645	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.27e-015	0.0173	0.00712	0.000577	0.000237
Water	2.07e-017	1.08e+003	325	36.1	10.8
Soil	8.73e-016	1.59e+003	0	53.1	0
Sediment	1.52e-017	0.432	0.0104	0.0144	0.000346

Persistence Time: 268 hr
Reaction Time: 300 hr
Advection Time: 2.47e+003 hr
Percent Reacted: 89.2
Percent Advected: 10.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 28.49
Water: 208.1
Soil: 208.1
Sediment: 832.3
Biowin estimate: 3.375 (days-weeks)

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

Reliability : (2) valid with restrictions
Data obtained through use of recognized model

Flag : Critical study for SIDS endpoint
18.12.2006 (3)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Deg. product :
Method : other
Year : 2004
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : BOD28/COD: 68%
COD: 1.26 g/g (O2)

Zahn-Wellen: 96%
The product is readily biodegradable.

Test substance : 2,2-bis(hydroxymethyl)propionic acid; purity 95-100%

Reliability : (4) not assignable
Safety data sheet; Insufficient details to evaluate reliability

02.01.2007 (6)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC0	:	> 5000
Method	:	other
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Harmless to fish up to the test concentration.
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity 95-100%
Reliability	:	(4) not assignable Safety data sheet; Insufficient details to evaluate reliability

02.01.2007 (6)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	
Exposure period	:	24 hour(s)
Unit	:	mg/l
EC50	:	= 38900
Method	:	other
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity 95-100%
Reliability	:	(4) not assignable Safety data sheet; Insufficient details to evaluate reliability

02.01.2007 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	
Endpoint	:	
Exposure period	:	7 day(s)
Unit	:	mg/l
EC3	:	= 16500
Method	:	other
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity 95-100%
Reliability	:	(4) not assignable Safety data sheet; Insufficient details to evaluate reliability

02.01.2007 (6)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 2000 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2004
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity 95-100%
Reliability	:	(2) valid with restrictions Provides basic data
Flag	:	Critical study for SIDS endpoint

22.12.2006 (6)

Type	:	LD50
Value	:	> 5000 - mg/kg bw
Species	:	
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	2,2-bis(hydroxymethyl)propionic acid; purity = 98%
Reliability	:	(4) not assignable Safety data sheet; Insufficient details to evaluate reliability

22.12.2006 (2)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535 and TA1537

Test concentration	:	0, 62, 185, 556, 1667, and 5000 ug/plate (used in Tests 1 and 2)
Cycotoxic concentr.	:	> 5000 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1998
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Also conducted in accordance with EEC protocol B.14 (Mutagenicity: Salmonella typhimurium, Reverse Mutation Assay) of the Council Directive 67/548/EEC Two independent bacterial reverse mutation assays using the plate incorporation method were conducted with five concentrations of the test substance, ranging from 62 - 5000 ug/plate. Negative vehicle (water) and positive controls were run simultaneously with the test substance.
Result	:	DMPA was not toxic to any of the strains, as evidenced by the absence of a drastic decrease in the mean number of revertant colonies. In both the absence and the presence of the S9 mix in all strains, DMPA did not cause a reproducible two-fold or greater increase in the mean number of revertant colonies appearing in the test plates compared to the background spontaneous reversion rate observed with the vehicle, and did not give evidence of a dose-response. The positive controls gave the expected increase in the number of his(+) revertants in both the absence (sodium azide, 9-aminoacridine, and 2-nitrofluorene) and the presence (2-aminoanthracene) of S9 mix.
Test substance	:	2,2-dimethylol propionic acid (DMPA)
Conclusion	:	It is concluded that the test substance DMPA was not mutagenic under the conditions used in this study.
Reliability	:	(1) valid without restriction Guideline study
Flag	:	Critical study for SIDS endpoint

15.12.2006 (7)

Type	:	Chromosomal aberration test
System of testing	:	Chinese hamster ovary cells
Test concentration	:	Test 1: 0, 1, 5, 10, 25, 50, 100, 200, 300, 400, 500, 750, 1000, and 1250 ug/ml Test 2: see methods
Cycotoxic concentr.	:	at 1250 ug/ml in the absence of S9 mix; at 1200 ug/ml and higher in the presence of S9 mix
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1998
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Also conducted in accordance with EEC protocol B.10 (Mutagenicity: in vitro Mammalian Cytogenetic test) of the Council Directive 67/548 Two independent chromosome aberration assays were conducted. The test substance was dissolved in Ham's F12 medium prior to testing. In the first assay in the absence and presence of S9 mix the treatment/fixation times were 18/18 and 3/18 h, respectively. In the second assay in the absence/presence of S9 mix the treatment/fixation times were: Absence of S9 mix: 18/18 h: 0, 300, 400, 500, 700, 800, 900, 1000, 1100, and 1200 ug/ml 32/32 h: 0, 25, 50, 100, 300, 400, 500, 700, 800, 900, 1000, and 1200 ug/ml

Presence of S9 mix:
3/18 h: 0, 500, 700, 800, 900, 1000, 1100, and 1200 ug/ml
3/32 h: 0, 300, 400, 500, 700, 800, 900, 1000, 1100, and 1200 ug/ml

The highest concentration tested was based on toxicity of the test substance to the cells. For each selected treatment, 200 well-spread metaphases per concentration (100 metaphases per culture) were analyzed by microscopic examination. Mitomycin C and cyclophosphamide were used as positive control substances in the absence and in the presence of the S9 mix, respectively.

Result : In neither chromosome aberration assay did DMPA, in the absence or in the presence of S9 mix, induce a reproducible, biologically relevant and statistically significant increase in the number of cells with structural chromosome aberrations at any of the concentrations and time points analyzed, when compared to the negative control values. An increase in the number of cells with endoreduplication was, however, observed at 700 ug/ml and higher at the 18 h harvest time in the presence of S9 mix. Endoreduplications are not structural aberrations and are not included in the final assessment of clastogenic activity. Treatment with the positive controls yielded the expected significant increase in the incidence of structural chromosome aberrations.

Test substance : 2,2-dimethylol propionic acid (DMPA)

Conclusion : It is concluded that the test substance DMPA was not clastogenic under the conditions used in this study.

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

22.12.2006 (8)

Type : Mammalian cell gene mutation assay

System of testing : cultured mouse lymphoma L5178Y cells

Test concentration : Test 1: 0, 0.1, 0.2, 0.4, 0.8, 1.6, 3.2, 4.2, 5.6, 7.5, and 10 mM; Test 2: 0, 0.625, 1.25, 2.5, 5 and 10 mM

Cycotoxic concentr. : > 10 mM

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 476

Year : 1998

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Method : Also conducted in accordance with EEC protocol (Gene Mutation Test - Mammalian cells In vitro) of Council Directive 87/302/EEC and US EPA "Health Effects Testing Guidelines 40 CFR 798.5300

Two TK assays were conducted. The test substance was dissolved in growth medium prior to testing. DMPA was not toxic to the L5178Y cells in both the absence and the presence of S9 mix. The highest concentration tested and evaluated was the limit dose of 10 mM. Methyl methanesulfphonate (MMS) and 3-methylcholanthrene (MCA) were used as positive control substances in the absence and in the presence of the S9 mix, respectively; growth medium without serum served as the negative vehicle control.

Result : In both assays DMPA did not induce a significant increase in mutant frequency at any dose level in the absence or presence of S9 mix. Treatment with the positive controls yielded the expected significant increase in mutant frequency compared to the negative controls.

Test substance : 2,2-dimethylol propionic acid (DMPA)

Conclusion : It is concluded that under the conditions used in this study, the test substance DMPA is not mutagenic at the TK-locus of mouse lymphoma L5178y cells.

Reliability : (1) valid without restriction
Guideline study

22.12.2006 (9)

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

(1) Aldrich Chemical Co. (2000) The 2000-2001 Aldrich Handbook of Fine Chemicals and Laboratory Equipment. (in ISHOW database)

(2) Aldrich Chemical Co., Inc. (1996) Safety Data Sheet for 2,2-Bis(hydroxymethyl)propionic, 98%. Product # 106615

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(6) Perstorp Specialty Chemicals AB (2004) Safety Data Sheet for Dimethylolpropionic Acid (reviewed 17.02.2004)

(7) TNO Nutrition and Food Research Institute (1998) Bacterial reverse mutation test with 2,2-dimethylol propionic acid (DMPA). Report number V98.692

(8) TNO Nutrition and Food Research Institute (1998) Chromosomal aberration test with with 2,2-dimethylol propionic acid (DMPA) in cultured Chinese hamster ovary cells. Report number V98.976

(9) TNO Nutrition and Food Research Institute (1998) Gene mutation test at the TK-locus of L5178Y cells with 2,2-dimethylol propionic acid (DMPA). Report number V98.864