FOREWORD INTRODUCTION

1,2-BUTANEDIOL

CAS N°: 584-03-2

Substance

End Point	:	**IDENTIFIERS, PHYSICAL AND CHEMICAL PROPERTIES**
Chemical Name	:	**1,2-Butanediol**
Common Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
RTECS Number	:	**EK0380000**

Synonyms

1,2-Butylene glycol **1,2-Dihydroxybutane**

Properties & Definitions

Molecular Formula	:	**C4H10O2**
Molecular Weight	:	**90.14**
Melting Point	:	**-50C***
Boiling Point	:	**193C**
State	:	**Liquid**
Vapour Pressure	:	**2.13kPa(16mmHg) at 100C**
Octanol/Water Partition Coefficient	:	**log Pow = -0.34 at 25C**
Water Solubility	:	**> 100g/l**
Impurities	:	**Water, 1,4-butanediol, 1-acetoxy-2-hydroxybutane**
General Comments	:	1,2-Butanediol is stable in neutral, acidic or alkaline solutions. *MP:(DCP) the value -40 to -30 is also reported.

Overall Evaluation

SHORT SUMMARY OF THE REASONS WHICH SUPPORT THE RECOMMENDATION

1,2-Butanediol is stable liquid, and the production volume was 882 tonnes for 1991 in Japan. This chemical is stable in acidic or alkaline solutions, and is classified as "readily biodegradable" by the results of the biodegradation test conducted as SIDS testing.

The chemical is non-toxic to fish, daphnids and algae.

The chemical showed no genotoxic effects, and NOAEL for repeated dose toxicity was 200 mg/kg/day and NOAEL for reproductive toxicity was 1,000 mg/kg/day. Estimated Dose of Low Concern (EDCL) was calculated as 0.2 mg/kg/day and 10 mg/kg/day for repeated dose toxicity and reproductive toxicity, respectively.

Daily intake of the chemical was estimated as 3.13E-4 mg/day from calculation using MNSEM 145J exposure model.

In conclusion, although 1,2-butanediol showed weak toxicity in toxicological tests, no further testing are needed at present.

Production-Trade

Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Geographic Area : **JPN**

Production

Quantity	*Year*
26000 T - P	**1985**
882 T - P	**1991**

General Comments : Data for 1985 is approximated and includes imported amounts.

References

!SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Processes

Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**

Process

Process comments : Production is done through a continuous reaction and distillation operation.

References

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Uses

Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Geographic Area : **JPN**

Use

Quantity	*Year*	*Comments*
		Industrial use in closed systems where the chemical is fully changed to other substances by esterification.

References

Secondary References : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point	:	**Pathway into the Environment and Environmental Fate.**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
Geographic Area	:	**JPN**

Quantity Transported

General Comments	:	1,2-Butanediol is used and transformed in closed systems so there is no emission and no exposure to the environment.

References

Secondary Reference	:	**!SIDSP***

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point	:	**CONCENTRATION**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
Geographic Area	:	**JPN**

Test Method and Conditions

Test method description : Multiphase, non-steady state equilibrium model for the evaluation of chemicals in the environment consisting of air , water, soil and sediment. Version 1.4.5J (presented by: Kikuo Yoshida) MNSEM 145J. Values are calculated.

Test Results

Matrix	*Concentrations*	*Spec.*	*Date*

AIR **2.42E-08 ppm**
In air, steady state mass = 1.78E-02g

AQ **1.43E-04 mg/l**
In water, steady state mass = 2.68E+06g

SOIL **7.11E-06 mg/l**
In soil, steady state mass = 1.14E+04g

SED **3.31E-04 mg/l**
In sediment, steady state mass = 3.31E+04g

FOOD **2.21E-11 mg/l**
In meat.

FOOD **2.18E-11 mg/l**
In milk.

PLANT **6.74E-05 mg/l**
In vegetation.

References

Primary Reference : **#URMEA***
Unpublished Report on Exposure Estimation Test conducted by MITI and Environmental Agency, Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 6-7, (1993)

Study

End Point	:	**HUMAN INTAKE AND EXPOSURE**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
Geographic Area	:	**JPN**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*
	AIR		**IHL**		
	AQ		**ORL**		
	FOOD		**ORL**		

Test Method and Conditions

Test method description : Multiphase, non-steady state equilibrium model for the evaluation of fate of chemicals in the environment consisting of air, water, soil and sediment. Version 1.4.5.J (presented by: Kikuo Yoshida) MNSEM 145J values are calculated.

Test Results

Intake	*Spec.*	*Date*

1.78E-06 mg/d
Inhalation of air (from MNSEM 145J)

2.86E-04 mg/d
Drinking water (from MNSEM 145J)

8.24E-07 mg/d
Ingestion of fish (from MNSEM 145J)

1.64E-12 mg/d
Ingestion of meat (from MNSEM 145J)

2.66E-12 mg/d
Ingestion of milk (from MNSEM 145J)

2.52E-05 mg/d
Ingestion of vegetable (from MNSEM 145J)

3.13E-04 mg/d
Total estimated exposure dose (from MNSEM 145J)

References

Primary Reference : **#URMEA***
Unpublished Report on Exposure Estimation Test conducted by MITI and Environmental Agency, Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 6, (1993)

Study

End Point	:	**BIODEGRADATION**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
Geographic Area	:	**JPN**
Species/strain/system	:	Activated sludge

Test Substance

Purity Grade	:	**99%**

Test Method and Conditions

Test method description	:	OECD Guideline 301C. GLP:YES. Aerobic test. The sludge samples were mixed by stirring in a single container, and then cultured at 25C for one month.

Test Results

Quantity		*Time*	*Comments on result*
32 %	AV		Degree of biodegradation from BOD7
81 %	AV		Degree of biodegradation from BOD14
96 %	AV		Degree of biodegradation from BOD28
92 %	AV		Degree of biodegradation from DOC
100 %	AV		Degree of biodegradation from HPLC

General Comments : These results indicate that 1,2-butylene glycol should be classified as "readily biodegradable".

References

Primary Reference : **#MITIR***
Chemical Report submitted by the Ministry of International Trade and Industry, Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 4, (1993)

Study

End Point	:	**PHOTODEGRADATION**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**

Test Substance

Purity Grade	:	**99%**

Test Method and Conditions

Test method description	:	W. J. Lyman et al., Handbook of Chemical Properties Estimation Method, McGraw Hill Book Co., 1981. GLP: No.

Test Results

Quantity	*Time*	*Comments on result*
		Half-life for photolysis: Infinitude 0.00D+00 mol/l/s (estimation)

References

Primary Reference :

#MITIR*

Chemical Report submitted by the Ministry of International Trade and Industry, Japan, (1993)

Secondary Reference :

!SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 5, (1993)

Study

End Point	:	**HYDROLYSIS**
Chemical Name	:	**1,2-Butanediol**
CAS Number	:	**584-03-2**
Study type	:	**LAB**
Medium	:	**AQ**
Specifications	:	**FRESH**

Test Substance

Purity Grade	:	**99%**

Test Method and Conditions

Test method description	:	OECD Guideline 111. GLP: YES. Hydrolysis measured as a function of pH.
Temperature	:	**25 C**
pH	:	**4-9**

Test Results

Quantity	*Time*	*Comments on result*
T/2	**>1 y**	Half lives of 1,2-butanediol at 25C and at pH 4.0, 7.0 and 9.0 equal or higher than 1 year.

References

Primary Reference :

#MITIR*

Chemical Report submitted by the Ministry of International Trade and Industry, Japan, (1993)

Secondary Reference :

!SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 5, (1993)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**

Species/strain/system : Swiss albino/ICR
Dose / Concentration : **>4192 mg/kg BW**
Exposure comments : Acute oral dosing for LD50 limit testing. The range of the doses was not provided.

Test Results

Organism	*Medium*	*Spec.*	*Route*	*Lifestage*	*Sex*	*Effect*	*Effect Comments*
MOUSE			**ORL**		**F**	**LD50**	

References

Primary Reference : **TXAPA9**
Holman, N. W. et al. Toxicology and Applied Pharmacology, 49, 385, (1979)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 10, (1993)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**

Species/strain/system : No information provided neither on strain nor on sex of the test rats.
Dose / Concentration : **>16000 mg/kg BW**

Test Results

Organism	*Medium*	*Spec.*	*Route*	*Lifestage*	*Sex*	*Effect*	*Effect Comments*
RAT			**ORL**	**ADULT**		**LD50**	

References

Primary Reference : **RTECS***
Registry of Toxic Effects of Chemical Substances

Secondary Reference : **!SIDSP***
Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 10, (1993)

Study

End Point : **MAMMALIAN TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
RAT			**ORL**	**ADULT**	**M**	**10/DOSE**	**10**
					F	**10/DOSE**	**10**

Species/strain/system : Crj-CD(SD) strain

Test Substance

Purity Grade : **>99%**
Vehicle - Solvent : Distilled water

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test. GLP:YES

Exposure

Exposure Period : **42 d**
Dose / Concentration : **40-1000 mg/kg BW**
Exposure comments : Daily oral gavage of 0 (negative control), 40, 200, or 1000mg/kg body weight/day for 42 days for males. Females were exposed from day 14 before mating to day 3 of lactation.

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	NOAEL			**M**	

200mg/kg body weight/day was the dose at which no toxic effects were observed.

EDLC

0.2mg/kg/day was calculated as estimated dose of low concern for repeated dose toxicity.

NEF

There were no death throughout the observation period of 42 days. Body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals did not show any visible differences.

SON FUNCT F
RESPI ACTIV

Transient hypolocomotion and hypopnea at the 1000mg/kg in females.

References

Primary Reference : **#MOMHW***
Chemical Report submitted by the Ministry of Health and Welfare, Japan

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 11-12, (1993)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
BACT			**VTR**				

Species/strain/system : Salmonella typhimurium: TA100, TA1535, TA98, TA1537

Test Substance

Purity Grade : **99%**
Vehicle - Solvent : DMSO

Test Method and Conditions

Test method description : Japanese Guideline for Screening mutagenicity testing of chemicals. 3 plates used per test. GLP:YES

Exposure

Dose / Concentration : **312.5-5000 ug/ PLATE**
Exposure comments : Doses of: 0, 312.5, 625, 1250, 2500 or 5000 micrograms of 1,2-butanediol were applied per plate in 3 plates. Positive control: A) S9 negative received AF-2 sodium azide or 9-aminoacridine, B) S9 positive received 2-aminoanthracene. S9 activated by phenobarbital and 5,6-benzoflavone.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
	CHNG				

Minimum concentration of test substance at which toxicity to bacteria was observed is > 5000ug/plate with metabolic activation and 5000ug/plate without metabolic activation.

DNA	**NEF**

In all strains at all concentrations tested, with or without metabolic activation, the test substance did not induce any changes within the chromosomal chromatin.

General Comments : 1,2-Butanediol was considered as "negative" in gene mutation tests under the experimental conditions used.

References

Primary Reference : **#MOMHW***
Chemical Report submitted by the Ministry of Health and Welfare, Japan

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 12-13, (1993)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
HAMST			**VTR**				

Species/strain/system : Chinese hamster CHL cells

Test Substance

Purity Grade : **>99%**
Vehicle - Solvent : DMSO

Test Method and Conditions

Test method description : Japanese Guideline for Screening mutagenicity testing of chemicals. Positive controls without S9 activation received mytomycin C and those with S9 activation received cyclophosphamide.

Exposure

Dose / Concentration : **0.23-0.90 mg/ml**

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	CELL				

The lowest concentration producing toxicity to cells with and without metabolic activation was > 1mg/ml.

DNA **NEF**

At all concentrations tested there were no chromosomal changes observed in the cells with or without metabolic activation as compared with negative controls.

General Comments : The test material (1,2-butanediol) was considered as negative in chromosomal aberration tests in vitro under the experimental conditions used.

References

Primary Reference : **#MOMHW***
Chemical Report submitted by the Ministry of Health and Welfare, Japan

Secondary Reference : **!SIDSP***
OECD/SIDS/MHW JAPAN. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 13-14, (1993)

Study

End Point : **REPRODUCTION**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
RAT			**ORL**	**ADULT**	**F**	**10/DOSE**	**10**
					M	**10/DOSE**	**10**

Species/strain/system : Crj-CD(SD) strain

Test Substance

Purity Grade : **>99%**

Test Method and Conditions

Test method description : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity Screening Test. GLP:YES

Exposure

Dose / Concentration : **40-1000 mg/kg BW**
Exposure comments : 1,2-Butanediol was given orally (gavage) at doses of 0, 40, 200, or 1000mg/kg body weight/day to female rats for 14 days before mating and continued through pregnancy up to 3 days of lactation. On day 4 of lactation all animals were sacrificed.

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
REPRO	**NEF**			**F**	

No reproductive toxicity observed in parental animals or offsprings. There were no visible differences in body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals.

NOAEL

1000mg/kg for parental and F1 generation.

REPRO **ELDC**

Estimated dose of low concern = 10 mg/kg/day

General Comments : There were no death throughout the entire observation period. There were no visible differences in body weight, food consumption, hematology parameters, clinical chemistry parameters, organ weight, or pathological examination between the treated and control animals. No effect on reproduction and developmental toxicities were observed.

References

Primary Reference : **#MOMHW***
Chemical Report submitted by the Ministry of Health and Welfare, Japan

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, 11-12, (1993)

Study

End Point : **AQUATIC ACUTE TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**

Species/strain/system : Red Killifish (Oryzias latipes)
Exposure Period : **24-96 h**
Exposure comments : Same doses were also tested for 48h and 72h.

Test Results

Organism	Medium	Spec.	Route	Lifestage	Sex	Effect	Effect Comments
FISH	**AQ**	**ESTUA**				**LC0** **LC50**	LC0 = 1000mg/l for 24h, 48h, 72h and 96h. LC50 > 1000mg/l for 24h, 48h, 72h, and 96h. (Both values reported as 1000ppm).

References

Primary Reference : **#URTEA***
Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : **AQUATIC ACUTE TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**

Species/strain/system : Water flea (Daphnia magna)
Exposure Period : **24 h**
Dose / Concentration : **100->1000 mg/l**

Test Method and Conditions

Test method description : Probit method

Test Results

Organism	Medium	Spec.	Route	Lifestage	Sex	Effect	Effect Comments
CRUS	**AQ**	**FRESH**				**LC0** **LC50**	Both values reported as 1000ppm.

References

Primary Reference : **#URTEA***
Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

Study

End Point : **AQUATIC TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
ALGAE	**AQ**	**FRESH**					

Species/strain/system : Green algae (Selenastrum capricornutum)

Test Substance

Purity Grade : **99%**

Test Method and Conditions

Test method description : OECD Guideline. GLP:NO

Exposure

Exposure Period : **72 h**

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	EC50				

Effective concentration (reported as EBC50) = 10,000ppm

References

Primary Reference : **#URTEA***
Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1991)

Study

End Point : **AQUATIC TOXICITY**
Chemical Name : **1,2-Butanediol**
CAS Number : **584-03-2**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
CRUS	**AQ**	**FRESH**					

Species/strain/system : Water flea (Daphnia magna)

Test Substance

Purity Grade : **99%**

Test Method and Conditions

Test method description : OECD Test Guideline. GLP: NO. Static test.

Exposure

Exposure Period : **21 d**

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
---	---	---	---	---	---
	NOEC				

Maximum concentration at which no effect was observed for 21 days > 1000mg/l. (Reported as 1000ppm).

References

Primary Reference : **#URTEA***
Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan, (1993)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)