FOREWORD INTRODUCTION

3-METHYL-2,3-PENTANEDIOL

CAS N°: 4457-71-0

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	4457-71-0
Chemical Name	3-Methyl-1,5-pentanediol
Structural Formula	$HOCH_2CH_2CHCH_2CH_2OH$ (with CH_3 on the central C)

RECOMMENDATIONS

The chemical is currently of low priority for further work.

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

A single oral administration of 3-methyl-1,5-pentanediol to rat induced ataxic gait and decreased locomotor activity only at 2,000 mg/kg [OECD TG 401]. Oral LD50 was greater than 2,000 mg/kg. There is no information available on skin irritation, eye irritation and skin sensitisation. In an OECD combined repeat dose and reproductive/developmental toxicity screening test [TG 422], male and female rats were received by gavage at doses of 0, 100, 300 and 1,000 mg/kg/day for at least 42 days. Salivation was observed in both sexes of 1,000 mg/kg. A lack of fat deposits and an increase of glycogen accumulation in the liver accompanied by increased liver weight were observed in the females of the 1,000 mg/kg dose group only. Based on these slight changes, NOAEL is considered to be 300 mg/kg/day. In the above study [OECD TG 422] this chemical showed no reproductive/developmental toxicity and the NOAEL is considered to be 1,000 mg/kg/day. Two kinds of *in vitro* genotoxicity studies, bacterial test [OECD TG 471] and mammalian test [OECD TG 473], show negative results with and without metabolic activation.

Environment

This chemical is readily biodegradable (67-95 % after 28 d), and bioaccumulation potential seems to be low based on Log Pow (-0.03). It is is hydrolytically stable between pH 4 to 9, but it is classified as "readily biodegradable". In the atmosphere, indirect photodegradation by the reaction with OH radical is expected with gaseous 3-methyl-1,5-pentanediol. The half-life is estimated to be 27 hours. A generic fugacity model (Mackey level III) shows this chemical would be distributed mainly to water.

According to a Japanese manufacturer, 0.1 kg/year of 3-methyl-1,5-pentanediol is released with 5.8 x 10^6 tonnes/year of effluent into inland sea. Local predicted environmental concentration (PEC_{local}) is 1.7 x 10^{-8} mg/l, employing the calculation model. The highest exposure to the general population via the environment would be expected through drinking water processed from surface water. The concentration in drinking water is assumed to be less than 1.7 x 10^{-8} mg/l.

3-Methyl-1,5-pentanediol has been tested in fish (*Oryzias latipes*), *Daphnia* and Algae (*Selenastrum capricornutum*). All acute and chronic values compiled in this report were ≥ 100 mg/L. Thus, this chemical does not seem to be hazardous to aquatic organisms.

A PNEC of 1 mg/L for the aquatic organisms was calculated from NOEC for alga (100 mg/L) using an assessment factor of 100.

Exposure

The production volume of 3-methyl-1,5-pentanediol in Japan was 2,000 tonnes in 1994, of which 1,800 tonnes was exported. This chemical is used as an intermediate in synthesis in the chemical industry.

Consumer Exposure is negligible, because 3-methyl-1,5-pentanediol is not contained in consumer products.

NATURE OF FURTHER WORK RECOMMENDED

No further work recommended.

FULL SIDS SUMMARY

CAS NO: 4457-71-0		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		OECD TG 102	< - 10 °C (freezing temperature)
2.2	Boiling Point		OECD TG 103	249 °C
2.3	Density		OECD TG 109	0.9708 g/cm^3 at 25 °C
2.4	Vapour Pressure		OECD TG 104	7.2E-2 Pa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	- 0.03 at 25 °C
2.6 A.	Water Solubility		OECD TG 105	Miscible at 25 °C
B.	pH			None
	pKa			None
2.12	Oxidation: Reduction Potential			None
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		Calculated	T1/2=27 h (5E5 molecules/cm3 OH)
3.1.2	Stability in Water		OECD TG 111	Stable at pH 4 ,7and 9 at 50°C
3.2	Monitoring Data			In air = None In surface water = None In soil/sediment = None In biota = None
3.3	Transport and Distribution		Calculated (Level III Fugacity Model)	(Release 100% to air) Air Water Soil Sediment 0.0% 41.4% 58.5% 0.2% (Release 100% to water) Air Water Soil Sediment 0.0% 99.6% 0.0% 0.4% (Release 100% to soil) Air Water Soil Sediment 0.0% 33.0% 66.9% 0.1%
			(local exposure)	PEC_{local} = None
3.5	Biodegradation		OECD TG 301C	Readily biodegradable
3.7	Bioaccumulation			None
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oryzias latipes*	OECD TG 203	LC_{50} (96h) >100 mg/L
			OECD TG 204	LC_{50} (14d) >100 mg/L
				NOEC (14d) >= 100 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	*Daphnia magna*	OECD TG 202	EC_{50} (24h, Imm) >1000 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD TG 201	EC_{50} (72h, Bms) >1000 mg/L
				NOEC (72hr) =100 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	*Daphnia magna*	OECD TG 211	EC_{50} (21d, Repro) >100 mg/L
				NOEC (21d, Repro) >= 100 mg/L

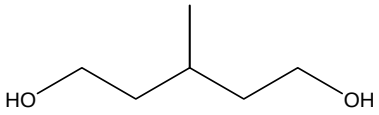
CAS NO: 4457-71-0		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	OECD TG 401	LD_{50} = > 2,000 mg/kg b.w.
5.2.1	Skin Irritation			No data
5.2.2	Eye Irritation			No data
5.3	Skin sensitization			No data
5.4	Repeated Dose Toxicity	Rat	OECD TG 422	NOAEL = 300 mg/kg/day
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	*S. typhimurium* *E. coli* WP2	OECD TG 471	- (With metabolic activation) - (Without metabolic activation)
B.	Non-Bacterial In Vitro Test (Chromosomal aberrations)	Chinese hamster CHL cells	Japanese TG and OECD TG 473	- (With metabolic activation) - (Without metabolic activation)
5.6	Genetic Toxicity In Vivo			No data
5.8	Toxicity to Reproduction	Rat	OECD TG 422	NOAEL = 1,000 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity	Rat	OECD TG 422	NOAEL = 1,000 mg/kg/day No teratogenicity
5.11	Experience with Human Exposure			None

SIDS INITIAL ASSESSMENT REPORT (SIAR)

3-Methyl 1,5-pentandiol

1. Identity

OECD Name: 3-Methyl-1,5-pentanediol
Synonym:
CAS Number: 4457-71-0
Empirical Formula: $C_6H_{14}O_2$
Structural Formula:



Degree of Purity: Unknown
Major Impurities: Unknown
Essential Additives: Unknown
Physical and chemical properties

	Protocol	Results
Melting Point	OECD TG 102	< - 10 °C (freezing temperature)
Densitity	OECD TG 109	0.9708 g/cm^3 at 25 °C
Vapour Pressure	OECD TG 104	7.2 x 10^{-2} Pa at 25 °C
Partition Coefficeint (Log Pow)	OECD TG 107	-0.03 at 25 °C
Water Solubility	OECD TG 105	Miscible at 25°C

2. Exposure

2.1 General discussion

The production volume of 3-methyl-1,5-pentanediol in Japan was 2,000 tonnes/year in 1994, of which 1,800 tonnes was exported.

3-methyl-1,5-pentanediol is hydrolytically stable at pH 4 to 9, but it is readily biodegradable (OECD 301C: 67-95 % after 28 days). In atmosphere, indirect photodegradation by the reaction with OH radical is expected with gaseous 3-methyl-1,5-pentanediol ($T_{1/2}$=27 hours).

2.2 Environmental exposure

a. Global exposure

The potential environmental distribution of 3-methyl-1,5-pentanediol obtained from a generic level III fugacity model under three emission scenarios is shown in Table 1. The results show that if 3-methyl-

1,5-pentanediol is released mainly to water, it is unlikely to distribute into other compartments. But, if 3-methyl-1,5-pentanediol is released mainly to air, it is likely to be transported both to water and soil.

Table 1 Environmental distribution of 3-methyl-1,5-pentanediol using a generic level III fugacity model under three emission scenarios

Compartment	Release: 100% to air	Release: 100% to water	Release: 100% to soil
Air	0.0%	0.0%	0.0%
Water	41.4%	99.6%	33.0%
Soil	58.5%	0.0%	66.9%
Sediment	0.2%	0.4%	0.1%

b. Local exposure

According to a Japanese manufacturer, 10 kg/year of 3-methyl-1,5-pentanediol are released into effluent treatment plant. 99% of it is removed in the plant and 1 % of it is released with 5.8×10^6 tonnes/year of effluent into inland sea. Local predicted environmental concentration (**PEC_{local}**) is 1.7×10^{-8} mg/l, employing the following calculation model. In this case, the dilution factor is estimated to be 1000.

$$\frac{\text{Amount of release } (1.0 \times 10^7 \text{ mg/y}) \times (1 - \text{Removal rate } (0.99))}{\text{Volume of effluent } (5.8 \times 10^9 \text{ l/y}) \times \text{Dilution factor } (1000)}$$

2.3 Consumer Exposure

3-Methyl-1,5-pentanediol is not contained in consumer products in Japan, because this chemical is used only in the intermediate in synthesis.

2.4 Exposure via the environment

The highest exposure to the general population via the environment would be expected through drinking water processed from surface water. Due to readily biodegradable nature of 3-methyl-1,5-pentanediol, a significant removal of during processing is expected. Although PEC_{global} cannot be estimated, the concentration in drinking water is assumed to be less than 4.7×10^{-8} mg/l.

2.5 Occupational exposure

- Occupational exposures at production sites may occur by the inhalation and dermal route.
- No actual workplace concentration data were available.
- Estimated exposure concentration by EASE model was 2.4-14 mg/m^3 as non-dispersive handling with local exhaust ventilation. The $EHE_{inhalaton}$ for w worker who operates drum filler for 3 hours a day without protective equipment was 0.77 mg/kg/day.
- Dermal exposure estimated using the EASE model for sampling work as non-dispersive, direct handling was 1-5 mg/cm^2/day. The EHE_{dermal} for 5 minutes sampling work was 0.63 mg/kg/day, assuming both hands were exposed.

- Based on these data, combined EHE was 1.4 mg/kg/day. Since workers always wear protective gloves and respiratory protective equipment (mask) during these operation, actual exposure could be lower.
- This substance is used as intermediate for polyurethane, polyester, plasticizer for epoxy resins.
- No occupational exposure limit for this chemical was located.

3 EFFECTS ON THE ENVIRONMENT

3.1 Toxicity to Aquatic Organisms

3-Methyl-1, 5-pentanediol has been tested in fish (*Oryzias latipes*), *Daphnia* and Algae (*Selenastrum capricornutum*). Results are summarized in Table 2. All data shown here were derived from the experiment conducted under GLP, and the chemical concentrations in the test media had been analyzed during the course of the experiments.

Table 2: Summary of effects of 3-Methyl-1,5-pentanediol on aquatic organisms

Organism	Test duration	Result (mg/L)	Reference
Aquatic plants, e.g. algae			
Green alga (*Selenastrum capricornutum*)	72 h (cl) 72 h (cl)	EC_{50} (Bms) >1000 (nc*) NOEC(Bms) =100 (nc*)	Japan EA (1997) Japan EA (1997)
Invertebrates			
Water flea (*Daphnia magna*)	24 h (s)	EC_{50} (Imm) >1000 (nc*)	Japan EA (1997)
	21 d (ss) 21 d (ss)	EC_{50} (Rep) >100 (nc*) NOEC(Rep) >= 100 (nc*)	Japan EA (1997) Japan EA (1997)
Fish			
Medaka (*Oryzias latipes*)	96 h (ss) 14 d (f)	LC_{50} >100 (nc*) LC_{50} >100 (nc*) NOEC >= 100 (nc*)	Japan EA (1997) Japan EA (1997)

cl = closed system
op = open system
f = flow through
s = static
ss = semi-static
nc* = calculated based on nominal concentrations, because measured concentrations were >80% of nominal concentrations
Bms = biomass
Imm = immobilization
Rep = reproduction

3.2 Toxicity to Terrestrial Organisms

There is no available information.

3.3 Other

There is no available information.

3.4 Initial Assessment for the Environment

This chemical is readily biodegradable (67-95 % after 28 d), and bioaccumulation potential seems to be low based on Log Pow (-0.03).

All acute and chronic data were =>100 mg/L. The predicted no effect concentration (PNEC) of 1 mg/L for the aquatic organisms was calculated from the NOEC for alga (100 mg/L, *Selenastrum*, 72 h, biomass) using an assessment factor of 100, because chronic data for fish were not available.

4. HUMAN HEALTH HAZARD

4.1 Effects on Human Health

a) Toxicokinetics and metabolism

There are no data available.

b) Acute toxicity

Two acute toxicity studies were reported for rat and mouse respectively. One is an oral rat study that was identified as the key study because it was well conducted and used a current protocol (OECD TG 401) in compliance with GLP [MHW, Japan: 1997]. The other is an intravenous mouse study, showing LD_{50} of 320 mg/kg [U.S. Army Armament Research & Development Command]. However the details were not reported.

Crj; CD (SD) rats received doses of 0, 1,000 and 2,000 mg/kg. No deaths occurred in both sexes. In the 2,000 mg/kg dose group, ataxic gait and decreased locomotor activity were observed in both sexes and in males, respectively. The oral LD_{50} value was more than 2000 mg/kg.

Human data

There are no data available.

Conclusions*:*

Oral LD_{50} of this chemical in rat is greater than 2,000 mg/kg.

c) Repeat dose toxicity

Only one study was found for repeat dose toxicity [MHW, Japan: 1997]. This study was identified as the key study because it was well conducted and used a current protocol in compliance with GLP. Details of the study are as follows.

In accordance with an OECD combined repeat dose and reproductive/developmental toxicity screening test [OECD TG 422], Crj: CD (SD) rats received 3-methyl-1,5-pentanediol by gavage at doses of 0, 100, 300 and 1,000 mg/kg/day. Males were dosed for 49 days and females were dosed from 14 days before mating, throughout pregnancy to day 3 of lactation.

In the 1,000 mg/kg group, salivation, which appeared immediately after dosing and lasted for about 1 hour, was observed in both sexes. Furthermore, a lack of fat deposits and an increase of glycogen accumulation in liver were recorded in females of 1,000 mg/kg group on histopathological examination by PAS staining. Those findings were associated with increased liver weights. In the

300 and 100 mg/kg, there were no effects of this chemical on general condition, body weights, food consumption, hematological and blood chemical parameters or histopathological findings. The NOAEL is considered to be 300 mg/kg/day.

There is no information available on humans.

Conclusions:

Based on clinical sign in both sexes and slight histopathological findings in female at 1,000 mg/kg, the NOAEL of repeat dose toxicity is considered to be 300 mg/kg/day.

d) Reproduction/developmental toxicity

The only available study is an OECD combined repeat dose and reproductive/developmental toxicity screening test [OECD TG 422]. This study was identified to be well conducted and reported [MHW, Japan: 1997].

3-Methyl-1,5-pentanediol was administered to Crj: CD (SD) rats by gavage at doses of 0, 100, 300 and 1,000 mg/kg from 14 days before mating to 14 days after mating in males and from 14 days before mating to day 3 of lactation in females.

There were no effects of this chemical on the estrous cycle, copulation index, fertility index, length of gestation, delivery, the gestation index, the number of corpora lutea and implantation sites or implantation index. With regard to the pups, there were no effects on the number of pups born, the number of dead pups, live birth index, sex ratio, external anomalies, viability index, body weight or necropsy findings. The NOAEL for reproductive/developmental toxicity is considered to be 1,000 mg/kg/day.

There is no information available on humans.

Conclusions:

There is no evidence that this chemical has any reproductive/developmental toxicity in rats. The NOAEL for the reproductive/developmental toxicity is considered to be 1,000 mg/kg/day.

e) Genotoxicity

Bacterial reverse mutation and chromosomal aberration tests from MHW are only available as the genotoxicity studies [MHW, Japan: 1997]. These studies were well conducted in compliance with a current protocol.

Baceterial in vitro test
Bacterial mutation test was conducted by Japanese TG and OECD TG 471, using *Salmonella typhimurium* TA100, TA1535, TA98 and TA1537, and *Escherichia coli* WP2 *uvr*A, with or without metabolic acitivation. All results were negative.

Non-bacterial in vitro test
Chromosomal aberration test by Japanese TG and OECD TG 473 was conducted in cultured Chinese hamster lung (CHL/IU) cells up to a maximum concentration of 1.2 mg/ml in continuous treatment, and short-term treatment with and without metabolic activation. Structual chromosomal aberrations and polyploidy were not induced in any assay conditions.

There is no information available on genotoxicity *in vivo*.

Conclusions:
Bacterial test and chromosomal aberration test *in vitro* showed negative results with and without metabolic activation.

f) Carcinogenicity

There are no data available.

g) Other human health related information

There are no data available for skin irritation, eye irritation and skin sensitisation.

4.2 Initial Assessment for Human Health

A single oral administration of 3-methyl-1,5-pentanediol to rat induced ataxic gait and decreased locomotor activity only at 2,000 mg/kg [OECD TG 401]. Oral LD_{50} was greater than 2,000 mg/kg. There is no information available on skin irritation, eye irritation and skin sensitisation. In an OECD combined repeat dose and reproductive/developmental toxicity screening test [TG 422], male and female rats were received by gavage at doses of 0, 100, 300 and 1,000 mg/kg/day for at least 42 days. Salivation was observed in both sexes of 1,000 mg/kg. A lack of fat deposit and an increase of glycogen accumulation in liver accompanying with increased liver weight were observed in only females of 1,000 mg/kg. Based on these slight changes, NOAEL is considered to be 300 mg/kg/day. In the above study [OECD TG 422] this chemical showed no reproductive/developmental toxicity and the NOAEL is considered to be 1,000 mg/kg/day. Two kinds of *in vitro* genotoxicity studies, bacterial test [OECD TG 471] and mammalian test [OECD TG 473], show negative results with and without metabolic activation.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Physical/chemical property, production, use and distribution
The production volume of 3-methyl-1,5-pentanediol in Japan is 2,000 tonnes in 1994, of which 1,800 tonnes was exported.. This chemical is used as intermediates in synthesis in chemical industry. This chemical is hydrolytically stable between pH 4 to 9, but it is classified as "readily biodegradable". In atmosphere, indirect photodegradation by the reaction with OH radical is expected with gaseous 3-methyl-1,5-pentanediol. The half-life is estimated to be 27 hours. A generic fugacity model (Mackey level III) shows this chemical would be distributed mainly to water.

According to a Japanese manufacturer, 0.1 kg/year of 3-methyl-1,5-pentanediol are released with 5.8×10^6 tonnes/year of effluent into inland sea. Local predicted environmental concentration (PEC_{local}) is 1.7×10^{-8} mg/l, employing the calculation model. The highest exposure to the general population via the environment would be expected through drinking water processed from surface water. The concentration in drinking water is assumed to be less than 1.7×10^{-8} mg/l.

Consumer Exposure is negligible, because 3-methyl-1,5-pentanediol is not contained in consumer products.

Environment

This chemical is readily biodegradable (67-95 % after 28 d), and bioaccumulation potential seems to be low based on Log Pow (-0.03).

3-Methyl-1,5-pentanediol has been tested in fish (*Oryzias latipes*) and *Daphnia* and alga (*Selenastrum capricornutum*). All acute and chronic values compiled in this report were >= 100 mg/L. Thus, this chemical does not seem to be hazardous to aquatic organisms.

PNEC of 1 mg/L for the aquatic organisms was calculated from NOEC for alga (100 mg/L) using an assessment factor of 100.

Human health

Oral LD_{50} value of 3-methyl-1,5-pentanediol in rats is greater than 2,000 mg/kg. There are no data available on skin irritation, eye irritation and skin sensitisation. In repeated dose toxicity study, the NOAEL is considered to be 300 mg/kg/day based on clinical sign and slight histopathological findings in 1,000 mg/kg. There is no evidence that this chemical has any reproductive/developmental toxicity in rats at 1,000 mg/kg/day. Bacterial test and chromosomal aberration test *in vitro* showed negative results with and without metabolic activation.

5.2 Recommendations

No recommendation

REFERENCES

Environment Agency of Japan (1997)

U.S. Army Armament Research & Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals. (Aberdeen Proving Ground, MD 21010), NX#01094.

Ministry of Health and Welfare: Japan (1997) *Toxicity Testing Reports of Environmental Chemicals* 5, 697-725.

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE 3 CHEMICAL

3-Methyl-1,5-pentanediol

CAS No. 4457-71-0

Sponsor Country: Japan

DATE: September, 2000

CONTENTS

2.11 OXIDISING PROPERTIES
2.12 † OXIDATION: REDUCTION POTENTIAL
2.13 ADDITIONAL REMARKS
A. PARTITION CO-EFFICIENT BETWEEN SOIL/SEDIMENT AND WATER (Kd)
B. OTHER REMARKS

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY
3.1.1 * PHOTODEGRADATION
3.1.2 * STABILITY IN WATER
3.1.3 STABILITY IN SOIL
3.2 * MONITORING DATA (ENVIRONMENT)
3.3 * TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS
3.3.1 TRANSPORT
3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)
3.4 MODE OF DEGRADATION IN ACTUAL USE
3.5 * BIODEGRADATION
3.6 BOD-5, COD OR RATIO BOD-5/COD
3.7 BIOACCUMULATION
3.8 ADDITIONAL REMARKS
A. SEWAGE TREATMENT
B. OTHER

4. ECOTOXICITY

4.1 * ACUTE/PROLONGED TOXICITY TO FISH
4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES
* A. DAPHNIA
B. OTHER AQUATIC ORGANISMS
4.3 * TOXICITY TO AQUATIC PLANTS e.g., ALGAE
4.4 TOXICITY TO BACTERIA
4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS
4.5.1 CHRONIC TOXICITY TO FISH
4.5.2 (*) CHRONIC TOXICITY TO AQUATIC INVERTEBRATES (e.g., DAPHNIA REPRODUCTION)
4.6 TOXICITY TO TERRESTRIAL ORGANISMS
4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS
4.6.2 TOXICITY TO TERRESTRIAL PLANTS
4.6.3 TOXICITY TO OTHER NON-MAMMALIAN TERRESTRIAL SPECIES (INCLUDING BIRDS)
4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)
4.8 BIOTRANSFORMATION AND KINETICS
4.9 ADDITIONAL REMARKS

5. TOXICITY

5.1 * ACUTE TOXICITY
5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY
5.1.3 ACUTE DERMAL TOXICITY
5.1.4 ACUTE TOXICITY BY OTHER ROUTES OF ADMINISTRATION
5.2 CORROSIVENESS/IRRITATION
5.2.1 SKIN IRRITATION/CORROSION
5.2.2 EYE IRRITATION/CORROSION
5.3 SKIN SENSITISATION
5.4 ***** REPEATED DOSE TOXICITY
5.5 ***** GENETIC TOXICITY IN VITRO
A. BACTERIAL TEST
B. NON-BACTERIAL IN VITRO TEST
5.6 ***** GENETIC TOXICITY IN VIVO
5.7 CARCINOGENICITY
5.8 ***** TOXICITY TO REPRODUCTION
5.9 ***** DEVELOPMENTAL TOXICITY / TERATOGENICITY
5.10 OTHER RELEVANT INFORMATION
A. SPECIFIC TOXICITIES (NEUROTOXICITY, IMMUNOTOXICITY etc.)
B. TOXICODYNAMICS, TOXICOKINETICS
5.11 ***** EXPERIENCE WITH HUMAN EXPOSURE

6. REFERENCES

Note: *; Data elements in the SIDS
†; Data elements specially required for inorganic chemicals

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. CAS-Number** 4457-71-0

B. Name (IUPAC name) 1,5-pentanediol, 3-Methy-

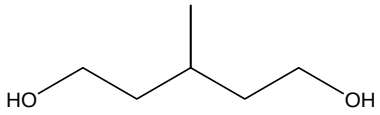
***C. Name** *(OECD name)* 3-Methy-1,5-pentanediol

†D. CAS Descriptor Not applicable

E. EINECS-Number 224-709-1

F. Molecular Formula $C_6H_{14}O_2$

***G. Structural Formula**



H. Substance Group Not applicable

I. Substance Remark None

J. Molecular Weight 118.18

1.02 OECD INFORMATION

A. Sponsor Country: Japan

B. Lead Organisation:

Name of Lead Organisation: Ministry of Health and Welfare (MHW)
Ministry of International Trade and Industry (MITI)
Environment Agency (EA)
Environment Agency (EA)
Ministry of Labor (MOL)

Contact person: Mr. Akitaka Saiki
Director
Second International Organization Bureau
Ministry of Foreign Affairs

Address: 2-2-1 Kasumigaseki, Chiyoda-ku
Tokyo 100, Japan
TEL 81-3-3581-0018
FAX 81-3-3503-3136

C. Name of responder

Name: Same as above contact person
Address:

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element **[ ]**; inorganic **[ ]**; natural substance **[ ]**;
organic **[X]**; organometallic **[ ]**; petroleum product **[ ]**

B. Physical State gaseous **[ ]**; liquid **[X]**; solid **[ ]**

C. Purity %

1.2 SYNONYMS 3-Methyl-1,5-pentanediol

1.3 IMPURITIES Unknown

1.4 ADDITIVES Unknown

***1.5 QUANTITY**

Location	Production	Date
Japan	2,000 tonnes/year	1994
	1,800 tonnes/year (export)	1994

Reference: MITI, Japan (1994)

1.6 LABELLING AND CLASSIFICATION

None

***1.7 USE PATTERN**

A. General

Type of Use:	Category:
main	Non dispersive use
industrial	Chemical Industry: used in synthesis
use	Intermediate

Reference: MITI, Japan (1994)

B. Uses in Consumer Products

None

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

None

*** 1.9 SOURCES OF EXPOSURE**

Source: Media of release: Water from a production site
Quantities per media: 0.1 kg/year

Remarks: 4-Metyl-1,5-pentanediol is produced in only one factory in Japan. 10 kg per year of it is released into a effluent treatment plant, where 99 % of it wad removed, and subsequently released into a inland sea.

Reference: MITI, Japan (1994)

1.10 ADDITIONAL REMARKS

A. Options for disposal

Reference:

B. Other remarks None

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT**

Value: < -10 °C
Decomposition: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Sublimation: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method: OECD TG 102 (Freezing temperature)
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Reference: MITI, Japan (1996)

***2.2 BOILING POINT**

Value: 249 °C
Pressure: OECD TG 103
Decomposition: Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Remarks: None
Reference: MITI, Japan (1996)

†2.3 DENSITY (Relative density)

Type: Bulk density **[ ]**; Density **[X]**; Relative Density **[ ]**
Value: 0.9708 g/cm^3
Temperature: 25 °C
Method: OECD TG 109
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Remarks: None
Reference: MITI, Japan (1996)

***2.4 VAPOUR PRESSURE**

Value: 7.2 x 10^{-2} Pa
Temperature: 25°C

Method:	calculated **[ ]**; measured **[X]** OECD Test Guideline 104 (Gas saturation method)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	None
Reference:	MITI, Japan (1996)

***2.5 PARTITION COEFFICIENT $log_{10}P_{ow}$**

Log Pow:	-0.03
Temperature:	25 °C
Method:	calculated **[ ]**; measured **[X]** OECD Test Guideline 107
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	None
Reference:	MITI, Japan (1996)

***2.6 WATER SOLUBILITY**

A. Solubility

Value:	
Temperature:	25 °C
Description:	Miscible **[X]**; Of very high solubility **[ ]**; Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[ ]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:	OECD Test Guideline 105
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	None
Reference:	MITI, Japan (1996)

B. pH Value, pKa Value

Not applicable

2.7 FLASH POINT

Value:	143 °C
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Reference:	Sigma-Aldrich company (1998)

2.8 AUTO FLAMMABILITY

No data available

2.9 FLAMMABILITY

Non-flammable based on flash point

2.10 EXPLOSIVE PROPERTIES

It can be predicted to be negative.

2.11 OXIDIZING PROPERTIES

It can be predicted to be negative.

2.12 OXIDATION: REDUCTION POTENTIAL

It can be predicted to be negative.

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

No data available

B. Other data

None

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.1 PHOTODEGRADATION

Type:	Air **[X]**; Water **[ ]**; Soil **[ ]**; Other **[ ]**
Light source:	Sun light **[ ]**; Xenon lamp **[ ]**; Other **[ ]**
Light spectrum:	. . . . . nm
Relative intensity:	
Spectrum of substance:	
Concentration of Substance:	
Temperature:	.
Indirect Photolysis:	
Type of sensitizer:	OH
Concentration of sensitizer:	
Rate constant (radical):	14.25 x 10^{-12} cm3/molecule*sec
Degradation:	50% after 27 hours
Method:	calculated **[X];** measured **[ ];**
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Substance grade, purity:not specified.
Remarks:	The reaction rate constant with OH radical was estimated by SRC AOPWIN v1.86. The half-life (27 hours) was calculated based on the calculated rate constant and OH radical concentration in atmosphere of 500000 molecules/cm^3.
Reference:	

*3.1.2 STABILITY IN WATER

Type:	Abiotic (hydrolysis) **[X]**; biotic (sediment)**[ ]**

Result:	Stable at pH 4, 7 and 9 at 25 °C
Method:	OECD Test guideline 111
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1,5-pentanediol
Remarks:	None
Reference:	MITI, Japan (1996)

3.1.3 STABILITY IN SOIL

No data available

*3.2 MONITORING DATA (ENVIRONMENT)

No data available

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

*3.3.1 TRANSPORT

No data available

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

The potential environmental distribution of 3-methyl-1,5-pentanediol obtained from a generic level III fugacity model under three emission scenarios is shown in Table and appendix 1. The results show that if 3-methyl-1,5-pentanediol is released mainly to water, it is unlikely to distribute into other compartments. But, if 3-methyl-1,5-pentanediol is released mainly to air, it is likely to be transported both to water and soil.

Environmental distribution of 3-methyl-1,5-pentanediol using a generic level III fugacity model.

Compartment	Release: 100% to air	Release: 100% to water	Release: 100% to soil
Air	0.0%	0.0%	0.0%
Water	41.4%	99.6%	33.0%
Soil	58.5%	0.0%	66.9%
Sediment	0.2%	0.4%	0.1%

Remarks:	None
Reference:	MITI, Japan (1996)

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

No data available

*3.5 BIODEGRADATION

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**;

Concentration of	100 mg/l related to Test Substance **[X]**
Medium:	water**[ ];**water-sediment**[ ];**soil **[ ];**sewage treatment **[ ]** other **[**Japanese standard activated sludge**]**
Degradation:	Degree of degradation after 28 days 80, 74 and 67 % from BOD 88, 85 and 74 % from TOC 93, 95 and 88 % from GC analysis
Results:	Readily biodeg. **[X];** Inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**
Method:	OECD Test Guideline 301 C
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1,5-pentanediol
Remarks:	None
Reference:	MITI, Japan (1996)

3.6 BOD_5, COD OR RATIO BOD_5/COD

Not applicable

3.7 BIOACCUMULATION

No data available

3.8 ADDITIONAL REMARKS

A. Sewage treatment None

B. Other information None

4. ECOTOXICOLOGICAL DATA

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

(a)

Type of test:	static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]** open-system **[ ]**; closed-system **[ ]**
Species:	*Oryzias latipes*
Exposure period:	96 hr
Results:	LC_{50} (24h) > 100 mg/L LC_{50} (72h) > 100 mg/L LC_{50} (96h) > 100 mg/L NOEC >= 100mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD Test Guideline 203 (1981)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1, 5-pentanediol (Wako Pure Chemical Industries), purity = 99.8%
Remarks:	A group of 10 fish were exposed to 1 nominal concentration (100 mg/L).
Reference:	EA, Japan (1997)

(b)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]** open-system **[ ]**; closed-system **[ ]**
Species:	*Oryzias latipes*
Exposure period:	14 days
Results:	LC_{50} (7d) > 100 mg/L LC_{50} (14d) > 100 mg/L LOEC > 100mg/L NOEC >= 100mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD Test Guideline 204 (1984)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1, 5-pentanediol (Wako Pure Chemical Industries), purity = 99.8%
Remarks:	A group of 10 fish were exposed to 5 nominal concentrations (6.25, 12.5, 25.0, 50.0 and 100 mg/L).
Reference:	EA, Japan (1997)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[ ]**; closed-system **[ ]**
Species:	*Daphnia magna*
Exposure period:	24 hr
Results:	EC_{50} (24h) > 1000mg/L EC_{50} (48h) > 1000mg/L NOEC >= 1000mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD Test Guideline 202 (1984)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1, 5-pentanediol (Wako Pure Chemical Industries), purity = 99.8%
Remarks:	20 daphnids (4 replicates; 5 organisms per replicate) were exposed to 1 nominal concentrations (1000 mg/L).
Reference:	EA, Japan (1997)

B. Other aquatic organisms

No data available

*4.3 TOXICITY TO AQUATIC PLANTS e.g. Algae

Species:	*Selenastrum capricornutum* ATCC 22662
End-point:	Biomass **[X]**; Growth rate **[X]**; Other **[ ]**
Exposure period:	72 hours
Results:	
Biomass:	EC_{50} (72h) >1000 mg/L NOEC (biomass) = 100 mg/L
Growth Rate:	EC_{50} (24h) >1000 mg/L

	EC_{50} (72h) >1000 mg/L
	NOEC (Growth Rate; 24 – 48 hours) >= 1000 mg/L
	NOEC (Growth Rate; 24 – 72 hours) >= 1000 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	open-system **[ ]**; closed-system **[ ]**
	OECD Test Guideline 201 (1984)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1, 5-pentanediol (Wako Pure Chemical Industries), purity = 99.8%
Remarks:	The EC_{50} values for biomass were calculated based on 3 nominal concentrations (100, 316 and 1000 mg/L).
Reference:	EA, Japan (1997)

4.4 TOXICITY TO BACTERIA

No data available

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1. CHRONIC TOXICITY TO FISH

No data available

(*)4.5.2. CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test:	static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	*Daphnia magna*
End-point:	Mortality **[ ]**; Reproduction rate **[X]**; Other **[ ]**
Exposure period:	21 days
Results:	
Reproduction:	EC_{50} (21 d) > 100 mg/L
	LC_{50} (21d) > 100 mg/L
	NOEC >= 1000 mg/L
	LOEC =
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD Test Guideline 202 (1984)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	3-Methyl-1, 5-pentanediol (Wako Pure Chemical Industries), purity = 99.8%
Remarks:	40 daphnids (4 replicates; 10 organisms per replicate) were exposed to each of 3 nominal concentrations (25, 50 and 100 mg/L).
Reference:	EA, Japan (1997)

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

(a)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Rat/Crj: CD (SD)
Value:	> 2,000 mg/kg Discriminating dose: 0, 1000, 2000 mg/kg
Method:	OECD Test Guideline 401
GLP:	Yes **[X]**; No **[ ]**; ? **[ ]**
Test substance:	purity: 99.18 %
Remarks:	No deaths occurred in males or females of both treatment groups. An ataxic gait was observed from 15 minutes to 2 hours after administration in males given 2000 mg/kg and from 15 to 30 minutes in females given 2000 mg/kg and decreased locomotive activity was observed for 30 minutes after administration in males given 2000 mg/kg. No effects were detected in terms of body weight changes or autopsy findings.
Reference:	MHW, Japan; 1997

5.1.2 ACUTE INHALATION TOXICITY

No data available

5.1.3 ACUTE DERMAL TOXICITY

No data available

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

(a)

Type:	LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[ ]** LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Mouse
Route of Administration:	i.m. **[ ]**; i.p. **[ ]**; i.v. **[X]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time:	No data available
Value:	320 mg/kg bw
Method:	Not specified
GLP:	Yes **[ ]**; No **[ ]**; ? **[X]**
Test substance:	purity: Unknown
Remarks:	Details of toxic effects not reported other than lethal dose value
Reference:	U.S. Army Armament Research & Development Command

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

No data available

5.2.2 EYE IRRITATION/CORROSION

No data available

5.3 SKIN SENSITISATION

No available data

*5.4 REPEATED DOSE TOXICITY (SIDS data)

(a)

Species/strain:	Rat/Crj: CD (SD)
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration:	Oral (by gavage)
Exposure period:	Males, 49 days Females, from 14 days before mating to the day before autopsy (day 3 of lactation)
Frequency of treatment:	Daily
Post exposure observation period:	1 day
Dose:	0 (Vehicle), 100, 300 and 1000 mg/kg/day
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOAEL:	300 mg/kg/day
Results:	In the 1000 mg/kg group, salivation, which appeared immediately after dosing and lasted for about 1 hour, was observed in approximately half of the animals, in males from day 29 of dosing and in females from day 10 of gestation. Further, disappearance of fat deposits and increased in glycogen accumulation in hepatocytes were recorded in females of the 1000 mg/kg group on histopathological examination. In the 300 and 100 mg/kg groups, there were no effects of administration of the test article on general condition, body weights, food consumption, hematological and blood chemical parameters or histopathological findings.
Method:	OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test (TG 422)
GLP:	Yes **[X]**; No **[ ]**; ? **[ ]**
Test substance:	purity: 99.18 %
Reference:	MHW, Japan; 1997

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

(a)

Type:	Bacterial reverse mutation assay
System of testing:	*Salmonella typhimurium* TA100, TA1535, TA98, TA1537, *Escherichia coli* WP2 *uvrA*
Concentration:	-S9 mix; 0, 313, 625, 1250, 2500, 5000 μg/plate (five strains) +S9 mix; 0, 313 - 5000 μg/plate (five strains)
Metabolic activation:	With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
S9:	Rat liver, induced with phenobarbital and 5,6-benzoflavone
Results:	Negative
Cytotoxicity conc:	With metabolic activation: Not observed Without metabolic activation: Not observed
Precipitation conc:	Precipitant was not found.

		+	?	-
Genotoxic effects:				
	With metabolic activation:	**[ ]**	**[ ]**	**[X]**
	Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 471
GLP: Yes **[X]**; No **[ ]**; ? **[ ]**
Test substance: purity: 99.18 %
Remarks: Positive controls: -S9 mix, 2-(2-Furyl)-3-(5-nitro-2-furyl) acrylamide (TA100, TA98, WP2), Sodium azide (TA1535) and 9-Aminoacridine (TA1537)
+S9 mix, 2-Aminoanthracene (five strains)
Reference: MHW, Japan; 1997

B. NON-BACTERIAL IN VITRO TEST

(a)
Type: Chromosomal aberration test
System of testing: Chinese hamster CHL/IU cells
Concentration: -S9 (continuous treatment): 0, 0.30, 0.60, 1.2 mg/ml
-S9 (short-term treatment): 0, 0.30, 0.60, 1.2 mg/ml
+S9 (short-term treatment): 0, 0.30, 0.60, 1.2 mg/ml
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
S-9: Rat liver, induced with phenobarbital and 5,6-benzoflavone
Results:
Cytotoxicity conc: With metabolic activation: Not observed
Without metabolic activation: Not observed
Precipitation conc: Precipitant was not found.

		clastogenicity			polyploidy		
		+	?	-	+	?	-
Genotoxic effects:	without metabolic activation:	**[ ]**	**[ ]**	**[X]**	**[ ]**	**[ ]**	**[X]**
	with metabolic activation:	**[ ]**	**[ ]**	**[X]**	**[ ]**	**[ ]**	**[X]**

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 473
GLP: Yes **[X]**; No **[ ]**; ? **[ ]**
Test substance: purity: 99.18 %
Remarks: Positive controls: -S9 mix, Mitomycin C
+S9 mix, Cyclophosphamide
Reference: MHW, Japan; 1997

5.7 CARCINOGENICITY

No data available

*5.8 TOXICITY TO REPRODUCTION

(a)
Type: Fertility **[ ]**; One-generation study **[X]**; Two-generation study **[ ]**; Other **[ ]**
Species/strain: Rats/ Cij;CD (Sprague-Dawley)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral (gavage)

Exposure period:	Male: 49 days Females, from 14 days before mating to the day before autopsy (day 3 of lactation)
Frequency of treatment:	Daily
Post exposure observation period: 1 day	
Premating exposure period: male: 14 days, female: 14 days	
Duration of the test:	Male; for 50 days, Female; 42-46 days
Doses:	0 (Vehicle), 100, 300 and 1000 mg/kg/day
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Corn oil Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOAEL Parental:	1000 mg/kg/day
NOAEL F1 Offspring:	1000 mg/kg/day
NOAEL F2 Offspring:	
Results:	There were no effects of administration of the test article on the estrous cycle, copulation index, fertility index, length of gestation, delivery, the gestation index, numbers of corpora lutea and implantation sites or implantation index. With regard to the pups, there were no effects of administration of the test article on the number of pups born, number of dead pups, live birth index, sex ratio, external anomalies, viability index, body weight or necropsy findings.
Method:	OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test (OECD TG 422)
GLP:	Yes **[X]**; No **[ ]**; ? **[ ]**
Test substance:	purity: 99.18 %
Reference:	MHW, Japan; 1997

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

No data available

5.10 OTHER RELEVANT INFORMATION

No data available

5.11 EXPERIENCE WITH HUMAN EXPOSURE

No data available

6. REFERENCES

Environment Agency of Japan (1997)
U.S. Army Armament Research & Development Command, Chemical Systems Laboratory, NIOSH Exchange Chemicals. (Aberdeen Proving Ground, MD 21010), NX#01094.
Ministry of Health and Welfare: Japan (1997) *Toxicity Testing Reports of Environmental Chemicals* 5, 697-725.
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MITI, Japan (1996): Unpublished data
Sigma-Aldrich company (1998) Sigma-Aldrich material Safety Data Sheets 11/1998 – 1/1999

Appendix 1 The potential environmental distribution of 3-methyl-1,5-pentanediol calculated based on a generic level III fugacity model under four emission scenarios

3-Methyl-1,5-pentanediol

Scenario 1

	emission rate	conc.	amount	percent	transfomation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	1,000	3.5.E-09	3.5.E+01	0.0	8.9E-01	3.5.E-01
water	0	2.1.E-02	4.2.E+05	41.4	2.4E+02	4.2.E+02
soil	0	3.7.E-01	5.9.E+05	58.5	3.4E+02	
sediment		1.6.E-02	1.6.E+03	0.2	3.0E-01	3.1.E-02
		total amount	1.0.E+06			

Scenario 2

	emission rate	conc.	amount	percent	transfomation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	0	3.8.E-15	3.8.E-05	0.0	9.7.E-07	3.8.E-07
water	1000	3.2.E-02	6.3.E+05	99.6	3.7.E+02	6.3.E+02
soil	0	4.0.E-07	6.4.E-01	0.0	3.7.E-04	
sediment		2.4.E-02	2.4.E+03	0.4	4.6.E-01	4.7.E-02
		total amount	6.4.E+05			

Scenario 3

	emission rate	conc.	amount	percent	transfomation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	0	6.9.E-13	6.9.E-03	0.0	1.8.E-04	6.9.E-05
water	0	1.8.E-02	3.6.E+05	33.0	2.1.E+02	3.6.E+02
soil	1000	4.6.E-01	7.4.E+05	66.9	4.3.E+02	
sediment		1.4.E-02	1.4.E+03	0.1	2.6.E-01	2.7.E-02
		total amount	1.1.E+06			

Scenario 4

	emission rate	conc.	amount	percent	transfomation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	600	2.1.E-09	2.1.E+01	0.0	5.4.E-01	2.1.E-01
water	300	2.4.E-02	4.8.E+05	52.6	2.8.E+02	4.8.E+02
soil	100	2.7.E-01	4.3.E+05	47.2	2.5.E+02	
sediment		1.8.E-02	1.8.E+03	0.2	3.4.E-01	3.6.E-02
		total amount	9.1.E+05			

Physicochemical parameters

molecular weight		118.17	Measured
melting point ［℃］		-10	Measured
vapor pressure [Pa]		7.20E-02	Measured
water solubility [g/m^3]		1000000	Measured
log Kow		0.03	Measured
half life [h]	in air	27	Estimated
	in water	1200	Estimated
	in soil	1200	Estimated
	in sediment	3600	Estimated

Temp. [℃]	25

Environmetal parameter

		volume [m^3]	depth [m]	area [m^2]	organic carbon [－]	lipid content [－]	density [kg/m^3]	residence time [h]
bulk air	air	1.0E+13					1.2	100
	particles	2.0E+03						
	total	1.0E+13	1000	1E+10				
bulk water	water	2.0E+10					1000	1000
	particles	1.0E+06			0.04		1500	
	fish	2.0E+05				0.05	1000	
	total	2.0E+10	10	2E+09				
bulk soil	air	3.2E+08					1.2	
	water	4.8E+08					1000	
	solid	8.0E+08			0.04		2400	
	total	1.6E+09	0.2	8E+09				
bulk sediment	water	8.0E+07					1000	
	solid	2.0E+07			0.06		2400	50000
	total	1.0E+08	0.05	2E+09				

Intermedia Transport Parameters ［m/h］

air side air-water MTC	5	soil air boundary layer MTC	5
water side air water MTC	0.05	sediment-water MTC	1E-04
rain rate	1E-04	sediment deposition	5E-07
aerosol deposition	6E-10	sediment resuspension	2E-07
soil air phase diffusion MTC	0.02	soil water runoff	5E-05
soil water phase diffusion MTC	1E-05	soil solid runoff	1E-08

PROPOSED ROBUST SUMMARY for

3-Methyl-1,5-pentanediol

PHYSICAL/CHEMICAL ELEMENTS

MELTING POINT

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method/guideline: OECD TG 102 (Freezing temperature)
- GLP: yes
- Year: 1996
- Remarks: None

RESULTS

- Melting point value: < -10 °C
- Decomposition: No
- Sublimation: No
- Remarks: None

CONCLUSIONS

Melting point is < -10 °C.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed:
- Order number for sorting
- Remarks:

BOILING POINT

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method: OECD TG 103 (Dynamic method)
- GLP: yes
- Year: 1996
- Remarks: None

RESULTS

- Boiling point value: 249 °C
- Pressure:
- Pressure unit:
- Decomposition: No
- Remarks: None

CONCLUSIONS

Boiling point is 249 °C.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed:
- Order number for sorting
- Remarks:

VAPOR PRESSURE

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method: OECD TG104 (Gas saturation method)
- GLP: yes
- Year: 1996
- Remarks: Vapour pressure was measured in triplicate at 60, 70 and 80 °C. The vapour pressure at 25 °C was calculated by extrapolating the linear regression equation between the logarithm of vapour pressure and the reciprocal of temperature

RESULTS

- Vapour Pressure value: 4.4, 3.6 and 3.4 Pa at 60 °C, 9.6, 6.4 and 9.2 Pa at 70 °C, 27, 24 and 23 Pa at 80 °C and 0.072 Pa at 25 °C (extrapolated value).
- Decomposition: no
- Remarks: Linear regression equation: log VP(Pa) = -4803.09 x (1/T) + 14.9657 (r = -0.981)

CONCLUSIONS

- The vapour pressure at 25 °C is 0.072 Pa.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed
- Order number for sorting
- Remarks:

PARTITON COEFFICIENT

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method: OECD TG 107 (Flask shake method)
- GLP: yes
- Year: 1996
- Remarks: After partition equilibrium of the test substance was established between n-octanol and water at three volume ratios, the concentrations of the test substance of both phases were determined with GC.

RESULTS

- Log P_{ow} -0.03
- Temperature: 25°C
- Remarks:
  Concentration in n-octanol and water phases under three conditions (mg/L):

Condition	Run 1		Run 2	
	Water phase	Octanol phase	Water phase	Octanol phase
1	287	310	288	317
2	282	312	288	310
3	279	301	280	296

CONCLUSIONS

- Log P_{ow} is -0.03.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed
- Order number for sorting
- Remarks:

WATER SOLUBILITY

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method: OECD TG 105 (Flask method)
- GLP: yes
- Year: 1996
- Remarks: 1 g of the test substance was added in duplicate to 1 ml of water in glass vessel. The solubility was visually checked.

RESULTS

- Value:
- Description of solubility: Very soluble
- pH value:
- pKa value:
- Remarks:

CONCLUSIONS

- Water solubility is miscible

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed
- Order number for sorting
- Remarks:

STABILITY IN WATER

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red spectroscopy.

METHOD

- Method/guideline: OECD TG 111
- Type: Hydrolysis as a function of pH
- GLP: yes
- Year: 1996
- Remarks: The hydrolysis was studied in duplicate at 1000 mg/L and at 50 °C for 5 days in each buffer of pH 4.0, 7.0 and 9.0 (preliminary test). The concentration of the test substance was determined with GC.

RESULTS

- Nominal concentration: 1000mg/L
- Measured value:
- Recovery % at pH 4.0, 7.0 and 9.0 at 50°C after 5 days: 101 and 103 % at pH 4.0, 92.4 and 94.0 % at pH 7.0, 108 and 105 % at pH 9.0
- Breakdown products: No
- Remarks: None

CONCLUSIONS

- 3-methyl-1,5-pentanediol is stable (half-life time >1 year) at pH 4.0, 7.0 and 9.0.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed
- Order number for sorting
- Remarks:

TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS (FUGACITY)

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks:.

METHOD

- Test (test type) Calculation
- Method: Fugacity level III
- Year: 1996
- Remarks:

RESULTS

- Media: air, water, soil and sediment
- Estimated Distribution and Media Concentration under three emission scenarios:

Compartment	Release 100% to air	Release 100% to water	Release 100% to soil
Air	0.0%	0.0%	0.0%
Water	41.4%	99.6%	33.0%
Soil	58.5%	0.0%	66.9%
Sediment	0.2%	0.4%	0.1%

- Remarks: None:

CONCLUSIONS

- Remarks: If 3-methyl-1,5-pentanediol is released mainly to water, it is unlikely to distribute into other compartments. But, if it is released mainly to air, it is likely to be transported both to water and soil.

DATA QUALITY

- Reliabilities: Reliable without restrictions, Key study
- Remarks:

REFERENCES (Free Text)

MITI, Japan

OTHER

- Last changed
- Order number for sorting
- Remarks:

BIODEGRADATION

TEST SUBSTANCE
- 3-Methyl-1,5-pentanediol (CAS No 4457-71-0)
- Remarks: Source:: Wako Pure Chemical Industries, Ltd. – purity: 99.8%, kept at 5 °C until use. The structure was identified by Infrared red, mass and nmr spectroscopies.

METHOD
- Method/guideline: OECD TG 301C
- Test Type: aerobic
- GLP: yes
- Year: 1996
- Contact time: 28 days
- Inoculum: activated sludge cultivated for OECD TG 301C
- Remarks: 30 mg of the test substance or aniline (reference substance) and 9 mg as MLSS of the activated sludge were added to 300 mL of test medium. The test and reference solutions were cultivated in BOD meter together with the inoculum blank and abiotic control ones at 25°C for 28 days, during which the oxygen consumption was continuously measured. After termination of the test, the total organic carbon concentration (TOC) of the test solution and the residual amount of the test substance were determined with TOC meter and GC, respectively. The biodegradability was calculated from the oxygen consumption, TOC and the residual amount.

RESULTS
- Degradation % after 28 days: 80, 74 and 67 % from BOD
  88, 85 and 74 % from TOC
  93, 95 and 88 % from GC
- Results: Ready biodegradable
- Kinetic: Biodegradability of the test substance from BDO: 7, 7 and 6 % after 7 days, 31, 31 and 28 % after14 days
  Biodegradability of the reference substance from BOD: 64 % after 7 days, 76 % after 14 days and 76 % after 28 days
- Breakdown products: no
- Remarks:

CONCLUSIONS
- This chemical is ready biodegradable

DATA QUALITY
- Reliabilities: Reliable without restrictions, Key study
- Remarks: Well conducted study, carried out by Chemicals Inspection & Testing Institute, Japan

REFERENCES (Free Text)
MITI, Japan

OTHER
- Last changed
- Order number for sorting
- Remarks:

ECOTOXICITY ELEMENTS

ACUTE TOXICITY TO FISH

TEST SUBSTANCE

• Identity: 3-Methyl-1,5-pentanediol

=> Remarks: Source: Wako Pure Chemical Industries - purity = 99.8 % (Lot. WDK5104)

METHOD

• **Method/guideline followed (experimental/calculated):** OECD Test Guideline 203 (1981)

• **Type (test type):** 96 hours mortality

• **GLP (Y/N):** Yes

• **Year (study performed):** 1996

• **Species/Strain/Supplier:** *Oryzias latipes* (Medaka); obtained from commercial hatcheries

• **Analytical monitoring:** The tested concentrations were measured at 0 hour and 48 hours (in advance of test solution exchange) by gas chromatography method.

• **Exposure period (h):** 96

• **Statistical methods:**

=> Remarks field for Test Conditions. Detail and discuss any significant protocol deviations, and detail differences from the guideline followed including the following as appropriate:

– Test fish (Age/length/weight, loading, pretreatment): length = 20 - 21 mm; weight = 0.13 - 0.15 g

– Test conditions, e.g.

· Details of test (static, semi-static, flow-through): Semi-static (water renewal: 48 hours)

· Dilution water source: Reconstituted water

· Dilution water chemistry (hardness, alkalinity, pH, DOC, TSS, salinity):

· Stock and test solution and how they are prepared: Not described

· Concentrations dosing rate, flow-through rate, in what medium: Concentrations of 100 mg/L were tested.

· Vehicle/solvent and concentrations: Not used

· Stability of the test chemical solutions: Not described

· Exposure vessel type (e.g., size, headspace, sealed, aeration, lighting, # per treatment): 2.5 L-test solution in a 3 L-glass vessel

· Number of replicates, fish per replicate: Number of replicates = 2; individuals per replicate = 5

· Water chemistry in test (O_2, pH) in the control and one concentration where effects were observed: pH 7.0 - 7.5; DO = 5.4 - 8.2 mg/L

· Lighting: 16:8 hours; light-darkness cycle

· Test temperature range: 23.8 - 24.5 °C

– Method of calculating mean measured concentrations (i.e. arithmetic mean, geometric mean, etc.):

RESULTS

• **Nominal concentrations (as mg/L):** 100

• **Measured concentrations (as mg/L):**

Nominal concentration (mg/L)	Measured concentration (mg/L) (Percentage of nominal)		
	0 hour	48 hours	Time-weighted mean
Control	n. d.	n. d.	n. d.
100	105(105)	101(101)	103(103)

n. d.: < 2.50 mg/L

• **Unit (results expressed in what unit):** mg/L

• Element value: LC_{50} at 96 hours > 100

• **Statistical results, as appropriate:** Not described

=> Remarks field for Results. Discuss if the effect concentration is greater than materials solubility. Describe additional information that may be needed to adequately assess data for reliability and use, including the following, if available:

– Biological observations: Not described

–Table showing cumulative mortality:

Nominal concentration (mg/L)	Cumulative number of dead fish (Percent mortality)		
	0 hour	24 hours	48 hours
	0(0)	0(0)	0(0)
Control	0(0)	0(0)	0(0)

– Lowest test substance concentration causing 100 % mortality:

– Mortality of controls: 0 % mortality during testing period.

– Abnormal responses: Not described

– Reference substances (if used) – results: LC_{50} (96 hours) = 0.945 mg/L for $Cu(II)SO_4 \cdot 5H_2O$

– Any observations, such as precipitation that might cause a difference between measured and nominal values.

CONCLUSIONS

=> Remarks field with the ability to identify source of comment, i.e. author and/or submitter

DATA QUALITY

• **Reliabilities:** Klimisch Code 1 = Reliable without restriction

=> Remarks field for Data Reliability

REFERENCES (Free Text)

Environmental Agency of Japan (1997)

OTHER

• Last changed (administrative field for updating)

• Order number for sorting (administrative field)

⇨ Remarks field for General Remarks (Use for any other comments necessary for clarification.)

TOXICITY TO AQUATIC PLANTS (E.G., ALGAE)

TEST SUBSTANCE

• Identity: 3-Methyl-1,5-pentanediol

=> Remarks: Source: Wako Pure Chemical Industries - purity = 99.8 % (Lot. WDK5104)

METHOD

• **Method/guideline followed (experimental/calculated):** OECD Test Guideline 201 (1984)
• **Test type (static/other):** Static
• **GLP (Y/N):** Yes
• **Year (study performed):** 1996
• **Species/strain # and source:** *Selenastrum capricornutum,* ATCC22662
• **Element basis:** The area below the growth curve
• **Exposure period:** 72 hours
• **Analytical monitoring:** The tested concentrations were measured by gas chromatography method.
• **Statistical methods:** Least squares method for EC, Dunnett test for NOEC

=> Remarks field for Test Conditions. Detail and discuss any significant protocol deviations and detail differences from the guideline followed including the following as appropriate:

– Test organisms
  · Laboratory culture
  · Method of cultivation: shaking culture (100 rpm)
  · Controls
– Test Conditions
  · Test temperature range: 23.2 - 23.8 °C
  · Growth/test medium: OECD medium
  · Shaking: 100 rpm
  · Dilution water source: Not applicable
  · Exposure vessel type: 100 ml-medium in a 500 ml-erlenmeyer flask with a silicon cap which allow ventilation
  · Water chemistry in test (pH) in at least one replicate of each concentration (at start and end of the test): pH in the inhibition test using *Selenastrum capricornutum* under static condition

Nominal concentration(mg/L)	pH	
	0 hour	72 hours
Control	8.1	10.0

100	8.1	10.2
316	8.1	9.6
1000	8.1	9.6

· Stock solutions preparation: No vehicle was used.
· Light levels and quality during exposure: 4200 - 4400 lux, continuous

–Test design:
· Number of replicates: Triplicate
· Concentrations: 100, 316 and 1000 mg/L
· Initial cell number in cells/ml: 1.0×10^4

– Method of calculating mean measured concentrations (i.e. arithmetic mean, geometric mean, etc.): Not described

RESULTS

• **Nominal concentrations in mg/L:** 100, 316 and 1000
• **Measured concentrations in mg/L:** n. d. for control, 101 – 102 for the nominal concentration of 100, 302 – 326 for the nominal concentration of 316, and 978 – 1030 for the nominal concentraion of 1000.

EbC_{50} (0 - 72 hours)	> 1000 mg/L
EbC_{50} (24 - 48 hours)	> 1000 mg/L
EbC_{50} (24 - 72 hours)	> 1000 mg/L
NOEC (biomass)	= 100 mg/L
NOEC (Growth Rate; 24 - 48 hours)	>= 1000 mg/L
NOEC (Growth Rate; 24 - 72 hours)	>= 1000 mg/L

• **Was control response satisfactory:** Yes (Cell density of 72 hours is over 100 times more than 0 hour, growth curves indicated the logarithmic growth during the test.)
• **Statistical results, as appropriate:** Not described

=> Remarks field for Results. Discuss if effect concentration is not less than materials solubility. Describe additional information that may be needed to adequately assess data for reliability and use including the following:

– Biological observations
· Cell density at each flask at each measuring point:

Nominal Concentration (mg/L)	Cell Density ($x10^4$ cells/mL) Mean(S.D.)				Growth Inhibition rate (%)
	0-hour	24-hour	48-hour	72-hour	
Control	1.0(0.0)	6.1(0.7)	34.8(2.0)	123.8(2.8)	-

100	1.0(0.0)	6.2(0.7)	36.7(0.9)	124.4(4.7)	-2.17
316	1.0(0.0)	5.7(0.6)	33.1(1.3)	108.7(4.9)	9.65
1000	1.0(0.0)	4.7(0.1)	27.9(0.8)	91.0(3.7)	24.7

· Growth curves: Logarithmic growth until end of the test
– Reference substances (if used) – results: LC_{50} (72 hours) = 0.358 mg/L for potassium dichromate

CONCLUSIONS

=> Remarks field with the ability to identify source of comment, i.e. author and/or submitter

DATA QUALITY

• **Reliabilities:** Klimisch Code: 1=reliable without restrictions

=> Remarks field for Data Reliability: Key study

REFERENCES (Free Text)

Environmental Agency of Japan (1997)

OTHER

• Last changed (administrative field for updating)
• Order number for sorting (administrative field)

⇨ Remarks field for General Remarks (Use for any other comments necessary for clarification.)

ACUTE TOXICITY TO AQUATIC INVERTEBRATES (E.G., DAPHNIA)

TEST SUBSTANCE

• Identity: 3-Methyl-1,5-pentanediol

=> Remarks: Source: Wako Pure Chemical Industries - purity = 99.8 % (Lot. WDK5104)

METHOD

• **Method/guideline:** OECD Test Guideline 202 (1984)
• **Test type:** 48 hours mortality test
• **GLP (Y/N):** Yes
• **Year (study performed):** 1996
• **Analytical procedures:** The tested concentrations were measured by gas chromatography method.
• **Species/Strain:** *Daphnia magna*
• **Test details:** Static
• **Statistical methods:** Not described

=> Remarks field for Test Conditions. Detail and discuss any significant protocol deviations and detail differences from the guideline followed including the following as appropriate:

– Test organisms:
· Source, supplier, any pretreatment, breeding method: Supplied from U.S. EPA Environmental Research Laboratory
· Age at study initiation: < 24 hours after hatching
· Control group: Not described

– Test conditions
· Stock solutions preparation and stability:
· Concentrations dosing rate, flow-through rate, in what medium: Concentrations of 1000 mg/L were tested
· Test temperature range: 20.0 - 20.1
· Exposure vessel type: Petri dish (diameter = 8.5 cm, depth = 5.7 cm)
· Dilution water source: Reconstituted water
· Dilution water chemistry: Not described
· Lighting: 16:8 hours; light darkness cycle
· Water chemistry in test:
DO and pH of test solutions during 48 hours static exposure of *Daphnia magna* to 3-methyl-1,5-pentanediol

Nominal concentration (mg/L)	Measured value			
	DO (mg/L)		pH	
	0 hour	48 hours	0 hour	48 hours
Control	8.8	8.4	8.0	7.6
1000	8.8	8.4	7.5	7.4

– Element (unit) basis: Immobility
– Test design: Number of replicates = 4; individuals per replicate = 5
– Method of calculating mean measured concentrations:
– Exposure period: 24 hours and 48 hours
– Analytical monitoring:

RESULTS

• **Nominal concentrations:** 1000 mg/L
• **Measured concentrations:** Measured concentration of 3-methyl-1, 5-pentanediol in acute immobilization test using *Daphnia magna* under static condition

Nominal concentration (mg/L)	Measured concentration (mg/L) (Percentage of nominal)		
	0 hour	48 hours	Time-weighted mean
Control	n. d.	n. d.	n. d.
1000	1040(104)	1010(101)	1030(103)

n. d. :<5.00 mg/L

• **Unit [results expressed in what unit]:** mg/L
• EC_{50} (24 hours, immobility) > 1000 mg/L; EC_{50} (48 hours, immobility) > 1000 mg/L; NOEC > 1000 mg/L;
• **Statistical results, as appropriate:** Not described

=> Remarks field for Results.

– Biological observations
· Number immobility as compared to the number exposed:

Nominal concentration (mg/L)	Cumulative number of immobilized *Daphnia* (Percentage immobility)	
	24 hours	48 hours
Control	0(0)	0(0)
1000	0(0)	0(0)

· Concentration response with 95% confidence limits: Not described
· Was control response satisfactory: Yes (No change is observed at pH and DO.)

– Reference substances (if used) – results: LC_{50} (48 hours) = 0.283 mg/L for potassium dichromate

CONCLUSIONS

=> Remarks field with the ability to identify source of comment, i.e. author and/or submitter

DATA QUALITY

• Reliabilities: Klimisch Code: 1 = Reliable without restriction

=> Remarks field for Data Reliability

REFERENCES (Free Text)

Environmental Agency of Japan (1997)

OTHER

• Last changed (administrative field for updating)
• Order number for sorting (administrative field)

=> Remarks field for General Remarks (Use for any other comments necessary for clarification.)

CHRONIC TOXICITY TO AQUATIC INVERTEBRATES (E.G., DAPHNIA)

TEST SUBSTANCE

• Identity: 3-Methyl-1,5-pentanediol

=> Remarks: Source: Wako Pure Chemical Industries - purity = 99.8 % (Lot. WDK5104)

METHOD

• **Method/guideline:** OECD Test Guideline 211
• **Test type:** 21 days reproduction test
• **GLP (Y/N):** Yes
• **Year (study performed):** 1996
• **Analytical procedures:** The tested concentrations were measured by gas chromatography method.
• **Species/Strain:** *Daphnia magna*
• **Test details:** Semi-static
• **Statistical methods:** Kruskal-Wallis test

=> Remarks field for Test Conditions. Detail and discuss any significant protocol deviations and detail differences from the guideline followed including the following as appropriate:

– Test organisms:
· Source, supplier, any pretreatment, breeding method: Supplied from U.S. EPA Environmental Research Laboratory
· Age at study initiation: < 24 hours after hatching
· Control group:

– Test conditions
· Stock solutions preparation and stability: Not used
· Test temperature range: 19.9 - 20.5
· Exposure vessel type: 0.8 L-test solution in a 1 L-glass vessel
· Dilution water source: Reconstituted water
· Dilution water chemistry: Not described
· Lighting: 16:8 hours; light darkness cycle
· Water chemistry in test: DO and pH of test solutions in reproduction test using *Daphnia magna* under semi-static condition

Nominal concentration (mg/L)	Measured value	
	DO (mg/L)	pH
Concentration	7.3 - 8.8	7.3 - 7.7

25.0	6.9 - 8.8	7.2 - 7.7
50.0	7.3 - 8.8	7.3 - 7.7
100	7.4 - 8.8	7.2 - 7.7

· Feeding: Daphids were fed green algae (*Chlorella vulgaris*); 0.1 - 0.2 mgC/day/individual

– Element (unit) basis: Reproduction
–Test design: Number of replicates = 4; individuals per replicate = 10
– Method of calculating mean measured concentrations (i.e. Time-weight arithmetic mean, geometric mean, etc.): Not described
– Exposure period: 21 days
– Analytical monitoring:

RESULTS

• **Nominal concentrations:** 25, 50 and 100 mg/L
• **Measured concentrations:**

Nominal concentration (mg/L)	Concentration of 3-metyl-1,5-pentanediol (mg/L)	
	Range	Mean
Control	n. d.	n. d.
25.0	23.2 - 25.7	24.4
50.0	45.9 - 51.7	49.6
100	96.3 - 106	102

n. d. :<5.00 mg/L

• **Unit [results expressed in what unit]:** mg/L
• EC_{50} > 100
LC_{50} (21 days) > 100
LOECr >= 100
NOECr >= 100
• **Statistical results, as appropriate:** Not described

=> Remarks field for Results.

– Biological observations
· Cumulative numbers of dead parental Daphnia:

Nominal concentration (mg/L)	Cumulative number of dead parental *Daphnia*		
	Exposure time (day)		
	7	14	21
0	0(0)	0(0)	0(0)

25.0	0(0)	0(0)	2(5.0)
50.0	0(0)	0(0)	0(0)
100	0(0)	0(0)	1(2.5)

The values in parenteses express mortality (%) of *Daphnia*.

· Time of the first production of young (d): 7 days
· Mean cumulative numbers of young produced per adult:

Nominal concentration (mg/L)	Mean cumulative numbers of young produced per adult at 21 days
0	86
25.0	102
50.0	109
100	99

· Was control response satisfactory: Yes

– Reference substances (if used) – results: LC_{50} (21 hours) = 0.283 mg/L for potassium dichromate

CONCLUSIONS

=> Remarks field with the ability to identify source of comment, i.e. author and/or submitter

DATA QUALITY

• **Reliabilities:** Klimisch Code: 1 = reliable without restrictions

=> Remarks field for Data Reliability

REFERENCES (Free Text)

Environmental Agency of Japan (1997)

OTHER

• Last changed (administrative field for updating)
• Order number for sorting (administrative field)

=> Remarks field for General Remarks (Use for any other comments necessary for clarification.)

HEALTH ELEMENTS

ACUTE TOXICITY

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No. 4457-71-0)

Remarks: Source: Kuraray Co. Ltd., Lot No. 63136, Purity: 99.18 %, Kept at room temperature and dark in nitrogen until use

METHOD

- **Method/guideline:** OECD TG 401
- **Test type:** Single dose toxicity test
- **GLP:** Yes
- **Year:** 1995
- **Species/ Strain:** Rat/ Crj; CD (SD)
- **Sex:** Male & Female
- **No of animals per sex per dose:** males, 5; females, 5/group
- **Vehicle:** None (without any dilution)
- **Route of administration:** Oral (gavage)

REMARKS FIELD FOR TEST CONDITIONS

- ***Age at study initiation*:** 6 weeks old for males and females
- ***Doses/concentration levels*:** 0 (water), 1000, 2000 mg/kg
- ***Post dose observation period:*** 14 days
- ***Weight at study initiation:*** 178-190 g for males, 136-145 g for females

RESULTS

- **LD_{50};** Male > 2,000 mg/kg, female > 2,000 mg/kg
- **No of deaths at each dose level;** No deaths at any dose levels

Remarks Field For Results.

- ***Body weight:*** No effect
- ***Clinical signs:*** An ataxic gait was observed from 15 minutes to 2 hours after administration in males given 2000 mg/kg and from 15 to 30 minutes in females given 2000 mg/kg and decreased locomotive activity was observed for 30 minutes after administration in males given 2000 mg/kg.
- ***Autopsy findings:*** No effects were detected

– ***Mortality and time to death:*** No deaths occurred during the study

CONCLUSIONS

No death occurred in males or females. An ataxic gait and decreased locomotive activity were observed. The rat oral LD_{50} value is over 2000 mg/kg for both sexes.

DATA QUALITY

- **Reliabilities:** Valid without restriction

Remarks field for Data Reliability

Well conducted study, carried out by Bozo Research Center Inc. (Japan)

REFERENCES (Free Text)

Ministry of Health and Welfare: Japan, Toxicity Testing Reports of Environmental Chemicals 5, 697-725 (1997)

GENERAL REMARKS

REPEATED DOSE TOXICITY

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No. 4457-71-0)

Remarks: Source: Kuraray Co. Ltd., Lot No. 63136, Purity: 99.18 %, Kept at room temperature and dark in nitrogen until use

METHOD

- **Method/guideline:** OECD TG 422
- **Test type:** OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
- **GLP:** Yes
- **Year:** 1995
- **Species:** Rat
- **Strain:** Crj; CD (SD)
- **Route of administration:** oral (by gavage)
- **Doses/concentration levels:** 0, 100, 300 and 1,000 mg/kg/day
- **Sex:** Male & Female
- **Exposure period:** Males; for 49 days
  Females; from 14 days before mating to the day before autopsy (day 3 of lactation)
- **Frequency of treatment:** Once daily
- **Control group and treatment:** Concurrent vehicle
- **Post exposure observation period:** 1 day
- **Duration of test:** Male; for 50 days
  Female; for 42-46 days
- **Statistical methods:** Dunnett's or Scheffe's test for continuous data and Chi square test for quantal data

Remarks Field For Test Conditions

– **Test Subjects:**

- ***Age at study initiation*:** 8 weeks old for males and females
- ***Weight at study initiation*:** 302-326 g for males, 206-232 g for females
- ***No. of animals per sex per dose*:** 12 per sex per dose group

– **Study Design:**

- ***Vehicle*:** Water
- ***Satellite groups and reasons they were added*:** none
- ***Clinical observations performed and frequency*:**
  General condition was observed once a day, body wt. and food consumption for males were weighed at day 1, 4, 8, 11, 15, 22, 29, 36, 43 and 50 of dosing.
  Hematology and biochemistry for males only at time of necropsy after 49 days of chemical exposure
- ***Organs examined at necropsy:***
  organ weight: thymus, heart, liver, spleen, kidney, testes, epididymis, ovary
  microscopic: for all the animals in control and 1000 mg/kg group: cerebrum, cerebellum, heart, liver, kidney, adrenal, testes, epididymis, infiltration and any organs which have gross pathological changes at necropsy. For females in 300 and 100 mg/kg: liver.

RESULTS

- **NOAEL**

300 mg/kg/day

Remarks Field For Results.

– ***Body weight:*** No effect
– ***Food/water consumption:*** No effect
– ***Clinical signs*** *(description, severity, time of onset and duration)**:***
Males/ Females: In the 1000mg/kg group, salivation, which appeared immediately after dosing and lasted for about 1 hour, was observed in approximately half of the animals, in males from day 29 of dosing and in females from day 10 of gestation.
– ***Haematology*:** No effect
– ***Biochemistry:*** No effect
– ***Ophthalmologic findings:*** Not examined
– ***Mortality and time to death:*** No deaths occurred during the study.
– ***Gross pathology incidence and severity:*** Dark red coloured deposits lying scattered in lung in one male rat and conglutinations in spleen, liver, stomach and adipose tissue around those organs in one female rat are observed in the 1000 mg/kg group.
– ***Organ weight changes:***
Female: increase in liver weight (absolute and relative) and in kidney weight (relative) at 1,000 mg/kg ($p<0.05$)

	females	
Dose level (mg/kg/day)	**0**	**1000**
Body weight (g, Mean ± SD)	351 ± 24	347 ± 20
Absolute weight		
Liver (g, Mean ± SD)	14.77 ± 1.50	16.90 ± 2.00**
Relative weight		
Liver (g%, Mean ± SD)	4.20 ± 0.24	4.87 ± 0.36**
Kidney (g%, Mean ± SD) right	0.32 ± 0.02	0.35 ± 0.02*
Kidney (g%, Mean ± SD) left	0.33 ± 0.02	0.35 ± 0.02*

– ***Histopathology*** *(incidence and severity)**:***
Female:
Liver: Lack of fat deposits and increased glycogen granule at 1,000 mg/kg

Dose level (mg/kg/day)	**degree***	**0**	**100**	**300**	**1000**
No. of animals		12	11	12	12
Fatty deposit/hepatocyte	0	2	6	6	12*
/periportal	1	10	6	6	0
	2	0	0	0	0
glycogen accumulation	0	4	3	4	0
/hepatocyte	1	8	9	8	4
	2	0	0	0	8*

*degree: 0 negative, 1 slight, 2 mild

CONCLUSIONS

In the 1,000mg/kg group, salivation, which appeared immediately after dosing and lasted for about 1 hour, was observed in approximately half of the animals, in males from day 29 of dosing and in females from day 10 of gestation. Furthermore, a lack of fat deposits and an increase of glycogen accumulation in hepatocytes were recorded in females of the 1,000 mg/kg group on histopathological examination. Based on clinical sign in both sexes and histopathological findings in female at 1,000 mg/kg, the NOAEL of repeat dose toxicity is considered to be 300 mg/kg/day.

DATA QUALITY

- **Reliabilities:** Valid without restriction

Remarks field for Data Reliability

Well conducted study, carried out by Bozo Research Center Inc. (Japan)

REFERENCES (Free Text)

Ministry of Health and Welfare: Japan, Toxicity Testing Reports of Environmental Chemicals 5, 697-725 (1997)

GENERAL REMARKS

This study was conducted to examine both repeated dose toxicity and reproductive/developmental toxicity as an OECD screening combined study. Therefore, biochemical and haematological analysis, and urinalysis for females were not performed. Functional observation and sperm examination were not performed because the test was conducted by the TG adopted in 1990

TOXICITY TO REPRODUCTION/DEVELOPMENT

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No. 4457-71-0)

Remarks: Source: Kuraray Co. Ltd., Lot No. 63136, Purity: 99.18 %, Kept at room temperature and dark in nitrogen until use

METHOD

- **Method/guideline:** OECD TG 422
- **Test type:** OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
- **GLP:** Yes
- **Year:** 1995
- **Species:** Rat
- **Strain:** Crj; CD (SD)
- **Route of administration:** oral (by gavage)
- **Doses/concentration levels:** 0, 100, 300, 1,000 mg/kg/day
- **Sex:** Male & Female
- **Exposure period:** Male; for 49 days from 2 weeks prior to mating
  Female; for 41-45 days from 2 weeks prior to mating to day 3 postpartum throughout mating and pregnancy
- **Frequency of treatment:** Once daily
- **Control group and treatment:** Concurrent vehicle
- **Post exposure observation period**: 1 day
- **Duration of test:** Male: for 50 days
  Female: for 42-46 days
- **Statistical methods:** Dunnett's or Scheffe's test for continuous data and Chi square test for quantal data

Remarks Field For Test Conditions

– **Test Subjects:**
  · ***Age at study initiation*:** 8 weeks old for males and females
  · ***Weight at study initiation*:** 302-326 g for males, 206-232 g for females
  · ***No. of animals per sex per dose*:** 12 per sex per dose group

– **Study Design:**
  The animals were sacrificed on the day 4 of lactation for females. Females with no delivery were killed on the day 25 of pregnancy.
  · ***Vehicle*:** Water
  · ***Satellite groups and reasons they were added*:** none
  · ***Mating procedures*:** Male/female per cage; 1/1, length of cohabitation; at the most 4 days, until proof of pregnancy (formation of vaginal closing or sperm detection in vagina)
  · ***Clinical observations performed and frequency*:**
  Parent: General appearance once a day
  Foetus: General appearance once a day after birth

Hematology, biochemistry and urinalysis for males only at time of necropsy after 49 days of chemical exposure

- ***Organs examined at necropsy*:**
  Parent: organ weight: thymus, heart, liver, spleen, kidney, testes, epididymis, ovary
  microscopic: all animals in control and 1000 mg/kg group: cerebrum, cerebellum, heart, liver, kidney, adrenal, testes, epididymis, infiltration and any organs which have gross pathological changes at necropsy. For females in 300 and 100 mg/kg: liver which have histopathological changes at the higher dose.
  Foetal: full macroscopic examinations on all of pups
- ***Parameters assessed during study*:**
  Body wt. (once a week), food/water consumption (once a week), No. of pairs with successful copulation, copulation index (No. of pairs with successful copulation/No. of pairs mated x 100), pairing days until copulation, No. of pregnant females, fertility index = (No. of pregnant animals/No. of pairs with successful copulation x 100), No. of corpora lutea, No. of implantation sites, implantation index (No. of implantation sites/No. of corpora lutea x 100), No. of living pregnant females, No. of pregnant females with parturition, gestation length, No. of pregnant females with live pups on day 0, gestation index (No. of females with live pups/No. of living pregnant females x 100), No. of pregnant females with live pups on day 4, delivery index (No. of pups born/No. of implantation sites x 100), No. of pups alive on day 0 of lactation, live birth index (No. of live pups on day 0/No. of pups born x 100), sex ratio (Total No. of male pups/Total No. of female pups), No. of pups alive on day 4 of lactation, viability index (No. of live pups on day 4/No. of live pups on day 0 x 100), body wt. of live pups (on day 0 and 4)

RESULTS

- **NOAEL**
  1,000 mg/kg/day

- **Actual dose received by dose level by sex if available:**
  0, 100, 300, 1000 mg/kg/day for both sexes

- **Reproductive data**

Dose level (mg/kg/day)		**0**	**100**	**300**	**1000**
No. of pairs mated		12	12	12	12
No. of pregnant females		11	12	12	12
No. of pregnant females with pups alive		11	12	12	12
Gestation index		100.0	100.0	100.0	100.0
Gestation length in days (Mean ± SD)		22.5 ± 0.5	22.7 ±0.5	22.7 ± 0.5	22.3± 0.5
Number of corpora lutea (Mean ± SD)		205(18.6 ±2.4)	230(19.2 ±1.5)	234(19.5 ± 3.1)	238(19.8 ± 2.6)
No. of implantations (Mean ± SD)		195(17.7 ± 2.3)	204(17.0 ± 1.9)	209(17.4 ± 2.1)	215(17.9 ± 1.4)
Implantation index		95.1	88.7	89.3	90.3
Day 0 of lactation					
No. of stillborn (Mean ± SD)		0(0.0 ±0.0)	3(0.3 ±0.5)	2(0.2 ± 0.4)	0.0(0.0 ±0.0)
No. of live born (Mean ± SD)		184(16.7 ± 2.0)	187(15.6 ±2.2)	195(16.3 ± 2.6)	201(16.8 ±1.9)
Delivery index		94.4	93.1	94.3	93.5
Live birth index		100	98.4	99.0	100
Sex ratio (Mean ± SD)		0.51	0.48	0.55	0.52
Day 4 of lactation					
Number of pups alive (Mean ± SD)		184(16.7 ± 2.0)	185(15.4 ±2.2)	189(15.8 ± 2.2)	197(16.4 ±1.8)
Viability index		100	98.9	96.9	98.0
Body weight of live pups (grams) (Mean ± SD)					
on day 0	**Males**	6.9 ± 0.8	7.2 ± 0.7	7.1 ± 0.7	6.71 ± 0.5
	Females	6.6 ± 0.7	6.7 ± 0.7	6.6 ± 0.7	6.3± 0.5
on day 4	**Males**	10.6± 1.7	11.0 ± 1.2	10.9 ±1.3	9.9 ± 0.9
	Females	10.3 ± 1.4	10.3 ± 1.2	10.3 ± 1.3	9.3 ± 0.9

Remarks Field For Results.

- ***Mortality and day of death*:** No deaths occurred during the study.
- ***Body weight**:* There were no effects on body weight.
- ***Food/water consumption:*** There were no effects on food/water consumption.
- ***Reproductive data*:** There were no statistically significant differences from controls.
- ***Fetal data*:** There were no statistically significant differences from controls.
- ***Grossly visible abnormalities, external, soft tissue and skeletal abnormalities*:** no statistically significant effects

CONCLUSIONS

There were no effects of administration of the test article on the estrous cycle, copulation index, fertility index, length of gestation, delivery, the gestation index, numbers of corpora lutea and implantation sites or implantation index. With regard to the pups, there were no effects of administration of the test article on the number of pups born, number of dead pups, live birth index, sex ratio, external anomalies, viability index, body weight or necropsy findings.
The NOAEL is considered to be 1,000 mg/kg/day for reproductive/developmental toxicity.

DATA QUALITY

- **Reliabilities:** Valid without restriction

Remarks field for Data Reliability

Well conducted study, carried out by Bozo Research Center Inc. (Japan)

REFERENCES (Free Text)

Ministry of Health and Welfare: Japan, Toxicity Testing Reports of Environmental Chemicals 5, 697-725 (1997)

GENERAL REMARKS

This study was conducted to examine both repeated dose toxicity and reproductive/developmental toxicity as an OECD screening combined study. Therefore, biochemical and haematological analysis, and urinalysis for females were not performed. Functional observation, anogenital distance and sperm examination were not performed because the test was conducted by the TG adopted in 1990.

GENETIC TOXICITY IN VITRO (BACTERIAL TEST)

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No. 4457-71-0)

Remarks: Source: Kuraray Co. Ltd., Lot No. 63136, Purity: 99.18 %, Kept at room temperature and dark in nitrogen until use

METHOD

- **Method/guideline**: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 471
- **Test type**: Reverse mutation assay
- **GLP***:* yes
- **Year**: 1995
- **Species/Strain:** *Salmonella typhimurium* TA100, TA1535, TA98, TA1537
  Escherichia coli WP2 uvr*A*
- **Metabolic activation:** With and without rat liver, induced with phenobarbital and 5,6-benzoflavone
- **Statistical methods**: No statistic analysis

Remarks Field For Test Conditions

– **Study Design:**
  - ***Concentration*:** -S9 mix; 0, 313, 625, 1250, 2500, 5000 μg/plate (five strains)
    +S9 mix; 0, 313, 625, 1250, 2500, 5000 μg/plate (five strains)
  - ***Number of replicates*:** 2
  - ***Plates/test*:** 3
  - ***Procedure*:** Pre-incubation method
  - ***Solvent*:** Water
  - ***Positive controls*:** -S9 mix, 2-(2-Furyl)-3-(5-nitro-2-furyl) acrylamide (TA100, TA98, WP2), Sodium azide (TA1535) and 9-Aminoacridine (TA1537)
    +S9 mix, 2-Aminoanthracene (five strains)

RESULTS

- **Cytotoxic concentration:**

Toxicity was not observed up to 5000 μg/plate in the five strains with or without S9 mix.

- **Genotoxic effects:**

	+	?	-
With metabolic activation:	**[ ]**	**[ ]**	**[X]**
Without metabolic activation:	**[ ]**	**[ ]**	**[X]**

Remarks Field For Results.

CONCLUSIONS

This chemical did not induce mutations in the *S. typhimurium* and *E. coli* strains with and without metabolic activation.

DATA QUALITY

- **Reliabilities:** Valid without restriction.

Remarks field for Data Reliability

Well conducted study, carried out by the Hatano Research Institute, Food and drug Safety Center (Japan)

REFERENCES (Free Text)

Ministry of Health and Welfare: Japan, Toxicity Testing Reports of Environmental Chemicals 5, 697-725 (1997)

GENERAL REMARKS

GENETIC TOXICITY IN VITRO (NON-BACTERIAL IN VITRO TEST)

TEST SUBSTANCE

- 3-Methyl-1,5-pentanediol (CAS No. 4457-71-0)

Remarks: Source: Kuraray Co. Ltd., Lot No. 63136, Purity: 99.18 %, Kept at room temperature and dark in nitrogen until use

METHOD

- **Method/guideline**: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 473

- **Test type**: Chromosomal aberration test

- **GLP***:* Yes

- **Year**: 1995

- **Species/Strain:** Chinese hamster lung (CHL/IU) cells

- **Metabolic activation:** Rat liver, induced with phenobarbital and 5,6-benzoflavone

- **Statistical methods**: Fisher's exact analysis

Remarks Field For Test Conditions

– **Study Design:**

· ***Concentration*****:** -S9 mix (continuous treatment): 0, 0.30, 0.60, 1.2 mg/ml
-S9 mix (short-term treatment): 0, 0.30, 0.60, 1.2 mg/ml
+S9 mix (short-term treatment): 0, 0.30, 0.60, 1.2 mg/ml
· ***Plates/test*****:** 2
· ***Solvent*****:** Distilled water
· ***Positive controls*****:** - S9, Mitomycin C
+ S9, Cyclophosphamide

RESULTS

- **Cytotoxic concentration:**

Toxicity was not observed up to 1.2 mg/ml in continuous and short-term treatment with or without S9 mix.

- **Genotoxic effects:**

	clastogenicity			polyploidy		
	+	?	-	+	?	-
– With metabolic activation:	**[ ]**	**[ ]**	**[X]**	**[ ]**	**[ ]**	**[X]**
– Without metabolic activation:	**[ ]**	**[ ]**	**[X]**	**[ ]**	**[ ]**	**[X]**

Remarks Field For Results.

CONCLUSIONS

Structural chromosomal aberrations and polyploidy were not induced in CHL/IU cells up to a maximum concentration of 1.2 mg/ml (10 mM) with continuous treatment, or with short-term treatment with and without an exogenous metabolic activation system.

DATA QUALITY

- **Reliabilities:** Valid without restriction

Remarks field for Data Reliability

Well conducted study, carried out by the Hatano Research Institute, Food and drug Safety Center (Japan)

REFERENCES (Free Text)

Ministry of Health and Welfare: Japan, Toxicity Testing Reports of Environmental Chemicals 5, 697-725 (1997)

GENERAL REMARKS