FOREWORD INTRODUCTION

2-HYDROXYPROPANENITRILE

CAS N°: 78-97-7

SIDS Initial Assessment Report
For
SIAM 2
(Paris, 4-6 July 1994)

Chemical Name: 2-Hydroxypropanenitrile

CAS No: 78-97-7

Sponsor Country: Japan

National SIDS Contact Point in Sponsor Country:
Mr. Yasuhisa Kawamura,
Ministry of Foreign Affairs, Japan

History: As a high priority chemical for initial assessment, 2-hydroxypropanenitrile was selected in the framework of the HPV Programme. At SIAM-2, the conclusion was approved with comments.

Comments at SIAM-2: Rearrangement of the documents.

Deadline for circulation:

Date of Circulation:

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	78-97-7
Chemical Name	2-Hydroxypropanenitrile
Structural Formula	CH_3-CH(OH)-CN

CONCLUSIONS AND RECOMMENDATIONS

It is currently considered of low potential risk and low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS

The production volume of 2hydroxypropanenitrile was ca. 11,000 tonnes/year in 1990 - 1993 in Japan. This chemical is used as an intermediate for the production of lactic acid, alanine, acrylic fibres and resins in closed systems in Japan. Also, it is used as and intermediate for acrylic acid and resins in Europe. This chemical is stable in neutral or acidic solutions, it is unstable in alkaline solution, and it is considered as "readily biodegradable".

PECs have been calculated based on fugacity level III models considering its physico-chemical properties (e.g. molecular weight, water solubility, vapour pressure and partition coefficient). The worst estimated concentrations were 7.0×10^{-8} mg/l (air), 6.7×10^{-5} mg/l (water), 3.7×10^{-4} mg/kg (soil), 1.2×10^{-4} mg/kg (sediment).

No monitoring data at the work place are available. As the chemical is used in closed systems, so far no data for consumer use are available. Based on the physico-chemical properties, the level exposed indirectly through the environment was estimated as 3.2×10^{-3} mg/man/day. The daily intake through drinking water is estimated as 1.3×10^{-4} mg/man/day and through fish is calculated as 2.2×10^{-6} mg/man/day.

For the environment, various NOEC and LC_{50} values were gained from test results; LC_{50} = 0.98 - 1.1 mg/l (acute fish); EC_{50} = 17 mg/l (acute daphnia); EC_{50} = 0.14 mg/l (acute algae); NOEC = 0.17 mg/l (long-term daphnia reproduction). Based on these values, the PNEC was estimated to be 0.0017 mg/l for aquatic organisms. Although the chemical is strongly toxic to fish and algae and moderately toxic to daphnids, PEC/PNEC ratio is less than 1. Therefore, it is considered to be of low risk for the environment.

Although the chemical showed no genotoxic effects in bacteria, weakly positive result was obtained in a chromosomal aberration test *in vitro*.

In a combined repeat dose and reproductive/developmental toxicity screening test, transient hypolocomotion, hypopnea and salivation were found at the highest dose (30 mg/kg/d) in both sexes. Increased liver weights occurred in the highest male group. In a pathological examination, enlargement of the liver was also observed in the same group. Such hepato-toxic effects were revealed to be due to a centrilobular hypertrophy and a fatty change of hepatocytes in a historical examination. For reproductive/developmental toxicity end-points, there were no effects observed concerning mating, fertility and oestrus cycle and also for dams during the pregnancy and lactation period. Therefore, NOEL was 6 mg/kg/day for repeated dose toxicity and 30 mg/kg/day for reproductive toxicity.

As for indirect exposure via environment, the daily intake through drinking water is estimated as 1.3×10^{-4}

mg/man/day and through fish is calculated as 2.2 x 10^{-6} mg/man/day. The margin of safety is very large. Therefore, health risk through the environment, in general, is considered to be low due to its use pattern and exposure situation.

In conclusion, no further testing is needed at present considering its toxicity and exposure levels.

NATURE OF FURTHER WORK RECOMMENDED

FULL SIDS SUMMARY

CAS NO: 78-97-7		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point			- 40 °C
2.2	Boiling Point			182 °C (at 1013 hPa)
2.3	Density			2.45 (relative density) at 20 °C
2.4	Vapour Pressure		OECD TG 104	1087 Pa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	- 0.32 at 25 °C
2.6 A.	Water Solubility		OECD TG 105	Infinite at 25 °C
B.	pH			No data available.
	pKa		OECD TG 112	Not observed.
2.12	Oxidation: Reduction Potential			No data available.
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		estimated	$T_{1/2}$ = 28.7 y (direct photodegradation in water)
3.1.2	Stability in Water		OECD TG 111	Stable at pH 4.0, 7.0. Half-life at pH 9.0 = 15.0 day at 25 °C
3.2	Monitoring Data			No data available.
3.3	Transport and Distribution		Calculated (MNSEM -147S)	In Air 7.0E-8 mg/L In Water 6.7E-5 mg/L In Soil 3.7E-4 mg/g In Sediment 1.2E-4 mg/g
3.5	Biodegradation		OECD TG 301C	Readily biodegradable: 56 - 76 % (BOD) 45 - 76% (TOC) and 100% (GC) in 28 days
3.6	Bioaccumulation	Carp	OECD TG 305C	BCF: 0.21
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oryzias latipes*	OECD TG 203	LC_{50} (72hr): 1.0 mg/L LC_{50}(96hr): 0.90 mg/L LC50(20d): 0.69 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50} (24hr): 17 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD TG 201	EC_{50} (72hr): 0.14 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50} (21d, Mortality): 0.71 mg/L NOEC(21d, Repro): 0.17 mg/L
4.6.1	Toxicity to Soil Dwelling			No data available.

CAS NO: 78-97-7		SPECIES	PROTOCOL	RESULTS
	Organisms			
4.6.2	Toxicity to Terrestrial Plants			No data available.
(4.6.3)	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)			No data available
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	OECD TG 401	LD_{50} : 31 mg/kg (male) 41 mg/kg (female)
5.1.2	Acute Inhalation Toxicity			LCLo: 124 ppm (4 hr)
5.1.3	Acute Dermal Toxicity			LD_{50} : 20 mg/kg
5.4	Repeated Dose Toxicity	Rat	OECD Combined Test	NOAEL = 6 mg/kg/day
5.5	Genetic Toxicity *In Vitro*			
A.	Bacterial Test (Gene mutation)	*S. .typhimurium* *E. coli*	OECD Guidelines No.471 and 472 and Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)	Negative (With metabolic activation) Negative (Without metabolic activation)
B.	Non-Bacterial *In Vitro* Test (Chromosomal aberrations)	CHL cells	OECD Guideline No.473 and Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)	Weakly positive (With metabolic activation) Weakly positive (Without metabolicactivation)
5.6	Genetic Toxicity *In Vivo*			No data available.
5.8	Toxicity to Reproduction	Rat	OECD Combined Test	NOAEL Parental = 30 mg/kg/day NOAEL F1 offspring = 30 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity			
5.11	Experience with Human Exposure			None

SIDS Initial Assessment Report

1. Identity

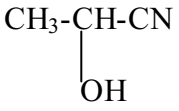
OECD Name: 2-Hydroxypropanenitrile

Synonym: Lactonitrile

CAS Number: 78-97-7

Empirical Formula: C_3H_5NO

Structural Formula:



Degree of Purity: 78.5 %

Major Impurities: free-CN 0.05 %, Aldehyde 0.05 %, water 21.1 %

Essential Additives: No additives

Physical-chemical Properties:

Melting Point:	-40 °C
Boiling Point:	182 °C
Density:	2.45
Vapor pressure:	1870 Pa at 25 °C
Water solubility:	infinite at 25 °C
Log Pow:	–0.32 at 25 °C

2. Exposure

2.1 General discussion

The production volume of 2-hydroxypropanenitrile was ca. 11,000 tonnes/year in 1990 - 1993 in Japan. This chemical is used as an intermediate for the production of lactic acid, alanine, acrylic fibres and resins in closed system in Japan. Also, it is used as an intermediate for acrylic acid and resins in Europe. All of disposal wastes are treated by incineration. Although this chemical is stable in neutral or acidic solutions, it is unstable in alkaline solution, and is classified as "readily biodegradable".

2.2 Environmental exposure

a) Biodegradability:

If released into water, this substance is readily biodegraded. In a MITI (I) test, corresponding to the OECD TG 301C: 56 - 66 % degradation during 28 days based on BOD, 45 -61 % based on TOC and 100% based on GC analysis was observed.

b) Hydrolysis as a function to pH:

The Half life of the test compound in pH 9 is 15.0 days and stable at pH 4 and 7.

c) Photodegradability (estimation)

The half-life time of 28.7 years is estimated for the direct photodegradation of lactonitrile in water by absorption of UV light (MITI, Japan).

d) Bioaccumulation:

A measured BCF of 0.21 in carp (6 weeks at 25 °C) suggests that the potential for bioconcentration in aquatic organisms is low.

e) Estimates of environmental fate, pathway and concentration:

PECs have been calculated based on several fugacity level III models (MNSEM, CHEMCAN, CHEMFRN) considering its physico-chemical properties (e.g. molecular weight, water solubility, vapour pressure and partition coefficient). The estimated concentrations of MNSEM model were 7.0 x 10^{-8} mg/l (air), 6.7 x 10^{-5} mg/l (water), 3.7 x 10^{-4} mg/kg (soil), 1.2 x 10^{-4} mg/kg (sediment). No monitoring data at work place and environment have been reported. The chemical is used in closed system, and no data for consumer use are available. Based on the physico-chemical properties, the total exposed dose indirectly through the environment was estimated as 3.2 x 10^{-3} mg/man/day. Also, the daily intake through drinking water is

estimated as 1.3 x 10^{-4} mg/man/day and through fish is calculated as 2.2 x 10^{-6} mg/man/day.

Global situation:

Method: MNSEM 147S

Input data:	Molecular weight:	71.08 [g/mole]
	Water solubility:	1000000 [mg/l]
	Vapor pressure:	1870 Pa [mmHg]
	Log Pow:	-0.32

Results: Steady state mass and concentration

Air:	7.0E-08 [mg/l]
Water:	6.7E-05 [mg/l]
Soil:	3.7E-04 [mg/kg dry solid]
Sediment:	1.2E-04 [mg/kg dry solid]

Environmental exposure dose (Concentration in foods)

Inhalation of air:	1.4E-03 [mg/day]
Drinking water:	1.3E-04 [mg/day]
Ingestion of fish:	2.2E-06 [mg/day]
meat:	1.1E-10 [mg/day]
milk:	1.8E-10 [mg/day]
vegetation:	1.6E-03 [mg/day]
Total exposure dose:	3.2E-03 [mg/day]

Table 1. Comparison of calculated environmental concentration using several models.

Model	Air[mg/l]	Water[mg/l]	Soil[mg/kg]	Sediment[mg/kg]
MNSEM	7.0E-08	6.7E-05	3.7E-04	1.2E-04
CHEMCAN2	3.6E-07	1.3E-04	9.8E-06	1.3E-06
CHEMFRAN	3.9E-08	2.1E-04	5.5E-06	2.1E-06

2.3 Consumer Exposure

No data on consumer exposure are available.

2.4 Occupational Exposure

No data on work place monitoring have been reported.

3. Toxicity

3.1 Human Toxicity

a) Acute toxicity

The oral LD50 value of lactonitrile for rats using OECD Test Guideline 401 is 87 mg/kg (MHW, Japan, 1993a). Also, the inhalation LCLo and the dermal LD50 are 124 ppm (4h) and 20 mg/kg, respectively.

b) Repeated toxicity

There is only one key study on repeated dose toxicity of lactonitrile. This chemical was studied for oral toxicity in rats according to the OECD combined repeated dose and reproductive/ developmental toxicity test [OECD TG 422]. As the study was well controlled and conducted under GLP, this was appropriate to regard as a key study. Male and female SD rats were orally administered (gavage) at doses of 0, 1.2, 6 and 30 mg/kg/day. In male rats, the administration period was two weeks prior to mating, 2 weeks of mating and 2 weeks after the completion of mating period. In female, in addition to maximum four weeks pre-mating and mating period, they were exposed through the pregnant period until day 3 of post delivery. Transient hypolocomotion, hypopnea, and salivation were found in the 30 mg/kg group of both sexes. There were no visible differences in body weight, food consumption, or hematological parameters between the treated and control animals of both sexes.
In an investigation of clinical chemistry parameters, a decrease in GOT and increase in total protein, albumin, and calcium were found in the 30 mg/kg group of males. Increased absolute and relative liver weights occurred in 30 mg/kg male group. In a pathological examination, enlargement of the liver was also observed in the 30 mg/kg group of males. This was revealed to be due to a centrilobular hypertrophy and a fatty change of hepatocytes in a histopathological examination. The NOEL for repeated dose toxicity was 6 mg/kg/day.

c) Reproductive toxicity

Lactonitrile was studied for oral toxicity in rats according to the OECD combined repeated dose and reproductive/developmental toxicity test [OECD TG 422] at doses of 0, 1.2, 6 and 30 mg/kg/day. Although this combined study was designed to investigate reproductive capability in parental generation as well as development in F1 offspring, parameters to evaluate developmental toxicity were limited to only body weights at day 0 and day 4 after birth, and autopsy findings at day 4. There were no effects on mating, fertility and oestrus cycle or on dams during the pregnancy and lactation period. External examination of pups revealed no increase in appearance of abnormal pups. Body weight gain of pups was normal. Pups killed

at postnatal day 4 showed no abnormal gross findings. NOEL for reproductive toxicity was 30 mg/kg/day.

d) Genetic toxicity

Bacterial test

A reverse gene mutation assay was conducted in line with Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Test Guidelines 471 and 472, using pre-incubation method. This study was well controlled and regarded as a key study. Lactonitrile showed negative results in *Salmonella typhimurium* TA100, TA1535, TA98, TA1537 and *Escherichia coli* WP2 uvrA at concentrations up to 1.5 mg/plate with or without metabolic activation system (MHW, 1993).

Non-bacterial test *in vitro*

A chromosomal aberration test in line with Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Test Guideline 473 was conducted using cultured Chinese Hamster lung (CHL/IU) cells. This study was well controlled and regarded as a key study. The maximum concentration of the chemical was used up to 0.71 mg/ml. Lactonitrile showed weak positive results with and without an exogeneous metabolic activation system (MHW, 1998).

in vivo test

No data are available on in vivo genotoxic effects.

e) Other human health related information

None

3.2 Ecotoxicity

Lactonitrile has been tested in a limited number of aquatic species (*Selenastrum capricornutum, Daphnia magna* and *Oryzias latipes*), under OECD test guidelines [OECD TG 201, 202, 203, 204 and 211]. Acute and chronic toxicity data to test organisms for 2-hydroxypropanenitrile are summarized in Table 2. No other ecotoxicological data are available. Various NOEC and LC50 values were gained from these tests; LC50(96h) = 0.90 mg/l (acute fish); EC50(24h) = 17 mg/l (acute daphnia); EC50(72h) = 0.14 mg/l (acute algae); 21d NOEC =0.17 mg/l (long-term daphnia reproduction). Therefore, the chemical is considered to be strongly toxic to fish and algae, and moderately toxic to daphnia. Applying an assessment factor of 100 to the lowest chronic toxicity data to daphnia (21 d-NOEC (reproduction) = 0.17 mg/l), a PNEC of 0.0017 mg/l is derived for lactonitrile. Since the PEC is lower than the PNEC, environmental risk is presumably low.

Table 2. Acute and chronic toxicity data of lactonitrile to aquatic organisms.

Species	Endpoint*1	Conc. (mg/L)	Reference
Selenastrum capricornutum (algae)	Biomass: EC_{50} (72h)	0.14 mg/L	MOE, Japan. (1992)
Daphnia magna (water flea)	Imm: EC_{50}(24h) Mor: EC_{50}(21d) Rep: EC_{50}(21d) Rep: NOEC	17 mg/L 0.71 mg/L 0.67 mg/L 0.17	
Oryzias latipes (fish, Medaka)	Mor: LC50(24h) Mor: LC0(72h) Mor:LC50(96h)	1.1 mg/L 1.0 mg/L 0.90 mg/L	
Fathead Minnow (fish)	Mor: LC50(20d)	0.69 mg/L	Henderson, et al., (1961)

Notes: *1 Mor; mortality, Rep; reproduction, Imm : Immobilisation

4. Initial Assessment

The production volume of 2-hydroxypropanenitrile was ca. 11,000 tonnes/year in 1990 – 1993 in Japan. This chemical is used as an intermediate for the production of lactic acid, alanine, acrylic fibres and resins in closed systems in Japan. It is also used as an intermediate for acrylic acid and resins in Europe. It is stable in neutral or acidic solutions, it is unstable in alkaline solution, and is considered as "readily biodegradable".

PECs have been calculated based on several models considering its physico-chemical properties (e.g. molecular weight, water solubility, vapour pressure and partition coefficient). The worst estimated concentrations were 7.0×10^{-8} mg/l (air), 6.7×10^{-5} mg/l (water), 3.7×10^{-4} mg/kg (soil), 1.2×10^{-4} mg/kg (sediment). No monitoring data at work place have been available. As the chemical is used in closed system, so far no data for consumer use are available. Based on the physico-chemical properties, the level exposed indirectly through the environment was estimated as 3.2×10^{-3} mg/man/day.

For the environment, various NOEC and LC50 values were gained from test results; 96h LC50 = 0.90 mg/l (acute fish); 24h EC50 = 17 mg/l (acute daphnia); 72h EC50 = 0.14 mg/l (acute algae); 21d NOEC = 0.17 mg/l (long-term daphnia reproduction). Based on these values, considering the test duration, the PNEC was estimated to be 0.0017 mg/l for aquatic organisms.
Although the chemical is strongly toxic to fish and algae and moderately toxic to daphnids, PEC/PNEC ratio is less than 1. Therefore, it is considered to be of low risk for the environment.

Although the chemical showed no genotoxic effects in bacteria, weakly positive results were obtained in a chromosomal aberration test in vitro. In a combined repeat dose and reproductive/developmental toxicity screening test, transient hypolocomotion, hypopnea and salivation were found at the highest dose (30 mg/kg/d) in both sexes. Increased liver weights occurred in the highest male group. In a pathological examination, enlargement of the liver was also observed in the same group. Such hepato-toxic effects were revealed to be due to a centrilobular hypertrophy and a fatty change of hepatocytes in a historical examination. Regarding reproductive/developmental toxicity end-points, there were no effects observed concerning mating, fertility and oestrus cycle and also for dams during the pregnancy and lactation period. Therefore, the NOEL was 6 mg/kg/day for repeated dose toxicity and 30 mg/kg/day for reproductive toxicity.

For indirect exposure via environment, the daily intake through drinking water is estimated as 1.3×10^{-4} mg/man/day and through fish is calculated as 2.2×10^{-6} mg/man/day. The margin of safety is very large. Therefore, health risk through the environment, is considered to be low due to its use pattern and exposure situation.

5. Overall recommendation and initial assessment

5.1 Conclusion

In conclusion, no further testing is needed at present considering its use pattern and degradability.

5.2 Recommendation

None

6. REFERENCES

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MITI, Japan: Unpublished data

MITI, Japan (1993) Unpublished Report (HPV/SIDS Test conducted by MITI, Japan. Test was performed in Chemicals Inspection and Testing Institute, Japan)

Sax (1989) Dangerous Properties of industrial Materials. Seventh Edition, Van Nostrand Reinhold

SIDS DOSSIER

2-Hydroxypropanenitrile

CAS No. 78-97-7

Sponsor Country : Japan

DATE: March, 2002

S I D S P R O F I L E

	CAS No.	78-97-7
1.01 C.	**CHEMICAL NAME (OECD Name)**	2-Hydroxypropanenitrile
1.01 D.	**CAS DESCRIPTOR**	Not applicable
1.01 G.	**STRUCTURAL FORMULA**	C_3H_5NO
	OTHER CHEMICAL IDENTITY INFORMATION	CH3-CH(OH)CN
1.5	**QUANTITY**	In Japan, approx 11,000 tonnes/year in 1990 - 1993.
1.7	**USE PATTERN**	In Japan, (a) Intermediate for lactic acid 80 % (b) Intermediate for alanine 20 % Closed system In European countries, intermediate for acrylic fibers and resins
1.9	**SOURCES AND LEVELS OF EXPOSURE**	In Japan, 1. Amount released from production site to water is negligible small. All of the waste water is incinerated 2. Amount released to air from production site is negligible. 3. Information on consumer exposure is not available.
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)		

S I D S S U M M A R Y

CAS NO: 78-97-7		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	SIDS Testing Required
STUDY		**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**
PHYSICAL-CHEMICAL DATA								
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.3	Density	Y	N	N	Y	N	Y	N
2.4	Vapour Pressure	N						Y
2.5	Partition Coefficient	N						Y
2.6	Water Solubility	N						Y
	pH and pKa values	N						N
OTHER P/C STUDIES RECEIVED								
ENVIRONMENTAL FATE and PATHWAY								
3.1.1	Photodegradation	N						Y
3.1.2	Stability in water	N						Y
3.2	Monitoring data	N						N
3.3	Transport and Distribution	N						N
3.5	Biodegradation	N						Y
3.6	Bioaccumulation	Y	Y	Y	N	N	Y	N
OTHER ENV FATE STUDIES RECEIVED								
ECOTOXICITY								
4.1	Acute toxicity to Fish	N						Y
4.2	Acute toxicity to Daphnia	N						Y
4.3	Toxicity to Algae	N						Y
4.5.2	Chronic toxicity to Daphnia	N						Y
4.6.1	Toxicity to Soil dwelling organisms	N						N
4.6.2	Toxicity to Terrestrial plants	N						N
4.6.3	Toxicity to Birds	N						N
OTHER ECOTOXICITY STUDIES RECEIVED								
TOXICITY								
5.1.1	Acute Oral	Y	N	N	Y	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	Y	N	Y	N
5.1.3	Acute Dermal	Y	N	N	Y	N	Y	N
5.4	Repeated Dose	N						Y
5.5	Genetic Toxicity *in vitro*							
	. Gene mutation	N						Y
	. Chromosomal aberration	N						Y
5.6	Genetic Toxicity *in vivo*	N						N
5.8	Reproduction Toxicity	N						Y
5.9	Development / Teratogenicity	N						Y
5.11	Human experience	N						N
OTHER TOXICITY STUDIES RECEIVED								

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

A.	**CAS-Number**	78-97-7
B.	**Name** (IUPAC name)	2-Hydroxypropanenitrile
C.	**Name** *(OECD name)*	Propanenitrile, 2-hydroxy-
D.	**CAS Descriptor**	Not applicable in this case
E.	**EINECS-Number**	201-163-2
F.	**Molecular Formula**	C_3H_5NO
G.	**Structural Formula**	CH3CH(OH)CN
H.	**Substance Group**	Not applicable
I.	**Substance Remark**	None
J.	**Molecular Weight**	71.08

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)

Contact person: Mr. Yasuhisa Kawamura
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 78.5 % (weight/weight)

1.2 SYNONYMS

Lactonitrile
2-Hydroxypropionitrile

1.3 IMPURITIES

(a) Name: free-CN
Value: 0.05 %
(b) Name: Aldehyde
Value: 0.05 %
(c) Name: Water
Value: 21.1 %

1.4 ADDITIVES None

1.5 QUANTITY

Location	Production(tonnes)	Date
Japan	11,000/year	1990-1993

1.6 LABELLING AND CLASSIFICATION

None

1.7 USE PATTERN

	Type of Use:	**Category:**
A. General	(a) main industry use	Intermediate for lactic acid (80 %) and alanine (20 %)

(b) main industry use Intermediate for acrylic fibers and resins

Remarks: None

Reference: (a) MITI, Japan
(b) ECDIN Database (1993)

B. Uses in Consumer Products

None

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

None

1.9 SOURCES OF EXPOSURE

(a)
Source: Media of release: Water from a production site
Quantities per media: < 1 kg/year
Remarks: All of the waste water is incinerated.
Reference: MITI, Japan
(b)
Source: Media of release: Air from a production site
Quantities per media: < 0.6 kg/year
Remarks: All of the waste gas in production process is incinerated.
References: MITI, Japan

1.10 ADDITIONAL REMARKS

A. Options for disposal: Incineration

Reference: MITI, Japan

B. Other remarks None

2. PHYSICAL-CHEMICAL DATA

2.1 MELTING POINT

Value:	- 40 °C
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	None
Reference:	Sax (1989)

2.2 BOILING POINT

(a)

Value:	103 °C
Pressure:	50 mmHg
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	None
Reference:	Sax (1989)

(b)

Value:	182 °C
Pressure:	760 mmHg
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	None
Reference:	ECDIN Database (1993)

2.3 DENSITY (Relative density)

Type:	Bulk density **[ ]**; Density **[ ]**; Relative Density **[X]**
Value:	2.45
Temperature:	20°C
Method:	Unknown
GLP:	Yes [ ] No **[ ]** ? **[X]**
Remarks:	None
Reference:	ECDIN database

2.4 VAPOUR PRESSURE

Value:	1870 Pa
Temperature:	25 °C
Method:	calculated **[ ]**; measured [X] OECD Test Guideline 104 Static Method
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	Purified substance (98%) used
Reference:	MITI, Japan (1993)

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

Log Pow:	- 0.32
Temperature:	25 °C
Method:	calculated **[ ]**; measured **[**X**]** OECD Test Guideline 107
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	None
Reference:	MITI, Japan (1993)

2.6 WATER SOLUBILITY

A. Solubility

Value:	Infinite
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:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	
Reference:	MITI, Japan (1993)

B. pH Value, pKa Value

No data available

2.7 FLASH POINT

Value:	170 °F
Type of test:	Closed cup **[ ]**; Open cup **[ ]**; Other **[X]**

Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	None
Reference:	Sax (1989)

2.8 AUTO FLAMMABILITY

No data available

2.9 FLAMMABILITY

Value:	Flame point: 89 °C
Results:	Extremely flammable**[ ]**;Extremely flammable-liquified gas**[ ]**; Highly Flammable **[ ]**; Flammable **[X]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	
Reference:	Bayer AG (1990)

2.10 EXPLOSIVE PROPERTIES

Results:	Explosive under influence of a flame**[ ]**; More sensitive to friction than m-dinitrobenzene **[ ]**; More sensitive to shock than m-dinitrobenzene **[ ]**; Not explosive **[ ]**; Other **[X]**
Method:	
GLP:	Yes **[ ]** No **[ ]** ? **[ ]**
Remarks:	No studies located, but not expected from structure to be explosive in temperature above flash point.
Reference:	ECDIN Database

2.11 OXIDIZING PROPERTIES

No studies located

2.12 OXIDATION: REDUCTION POTENTIAL

No studies located

2.13 ADDITIONAL DATA

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

No studies located

B. Other data None

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

3.1.1 PHOTODEGRADATION

Type:	Air **[ ]**; Water **[X]**; Soil **[ ]**; Other **[ ]**	
Light source:	Sun light **[X]**; Xenon lamp **[ ]**; Other **[ ]**	
Light spectrum:		
Relative intensity:		
Spectrum of substance:	epsilon =	6.75 at 300 nm
Concentration of Substance:		
Estimated parameter for calculation:		
	Quantum yield:	0.01
	Concentration:	5×10^{-5} M
	Depth of water body:	500 cm
	Conversion rate:	6.023×10^{20}
Results:	Degradation rate:	3.82×10^{-14}mol/l/s
	Half life:	28.7 years
Reference	Lyman et al. (1981)	

3.1.2 STABILITY IN WATER

Type:	Abiotic (hydrolysis) **[X]**; biotic (sediment)**[ ]**
Half life:	15.0 day at pH 9 at 25 °C Not hydrolysed at pH 4 and 7
Method:	OECD Test Guideline 111
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	2-Hydroxypropanenitrile, purity: > 99 %
Remarks:	None
Reference:	MITI, Japan (1993)

3.1.3 STABILITY IN SOIL

No studies located

3.2 MONITORING DATA (ENVIRONMENT)

No studies located

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

3.3.1 TRANSPORT No studies located

3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[ ]**; Soil-biota **[ ]**; Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**; Other **[X]** (Air-soil-water- sediment)

Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[X]**; Fugacity level IV **[ ]**; Other(calculation) **[ ]**; Other (measurement)**[ ]**

Results: Steady state mass and concentration calculated using MNSEM 147S

Air:	7.0E-08 [mg/l]
Water:	6.7E-05 [mg/l]
Soil:	3.7E-04 [mg/kg dry solid]
Sediment:	1.2E-04 [mg/kg dry solid]

Exposure dose

Inhalation of air:	1.4E-03 [mg/day]
Drinking water:	1.3E-04 [mg/day]
Ingestion of fish:	2.2E-06 [mg/day]
meat:	1.1E-10 [mg/day]
milk:	1.8E-10 [mg/day]
vegetation:	1.6E-03 [mg/day]

Total exposure dose: 3.2E-03 [mg/day]

Remarks: Input data:

Molecular weight:	71.08
Water solubility:	1000000 [mg/l]
Vapor pressure:	1,087 Pa [mmHg]
Log Pow:	-0.32

MNSEM 147S is a slightly revised version of MNSEM 145I.

1. addition of air particle compartment to air phase
2. execution of calculation on a spreadsheet program

Table 1. Comparison of calculated environmental concentration using several methods (Japanese environmental conditions are applied to the calculations.)

Model	Air[mg/l]	Water[mg/l]	Soil[mg/kg]	Sediment[mg/kg]
MNSEM	7.0E-08	6.7E-05	3.7E-04	1.2E-04
CHEMCAN2	3.6E-07	1.3E-04	9.8E-06	1.3E-06
CHEMFRAN	3.9E-08	2.1E-04	5.5E-06	2.1E-06

Reference: EA & MITI, Japan (1993)

3.4 IDENTIFICATION OF MAIN MODE OF DEGRADABILITY IN ACTUAL USE

No studies located.

3.5 BIODEGRADATION

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; activated sludge, 30 mg/l as suspended solid
Concentration of the chemical:	100 mg/l related to COD **[ ]**; DOC **[ ]**; Test substance **[X]**;
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment others [X] (Japanese standard activated sludge)
Degradation:	Degree of degradation after 28 days 56, 76 and 66 % from BOD 5, 71, 76 % from TOC analysis 100, 100 and 100 % from GC analysis
Results:	Readily biodeg. **[X];** Inherently biodeg. **[ ];** under test condition no biodegradation observed **[ ]**, Other **[ ]**
Method:	OECD TG 301C
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	2-Hydroxypropanenitrile, purity: > 99 %
Remarks:	None
Reference:	MITI, Japan (1993)

3.6 BOD_5,COD OR RATIO BOD_5/COD

Not applicable

3.7 BIOACCUMULATION

Species:	Carp
Exposure period:	6 weeks
Temperature:	25 °C
BCF:	0.21
Elimination:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	OECD TG 305C
Type of test:	**[ ]** calculated; **[X]** measured static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Lactonitrile
Remarks:	None
Reference:	MITI, Japan (1993)

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 **[X]**; closed-system **[ ]**
Species: *Oryzias latipes*
Exposure period: 96 hr
Results: $LC_{50\ (24h)}$ = 1.1 mg/l (95% confidence level: 0.3-3.5 mg/l)
$LC_{50\ (48h)}$ = 1.0 mg/l (95% confidence level: 0.4-2.2 mg/l)
$LC_{50\ (72h)}$ = 1.0 mg/l (95% confidence level: 0.4-2.2 mg/l)
$LC_{50\ (96h)}$ = 0.98 mg/l (95% confidence level: 0.7-1.2 mg/l)
NOEC =
LOEC =
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD Test Guideline 203 (1981)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: 2-Hydroxypropanenitrile, purity = 92.3 %
Remarks: A group of 10 fishes were exposed to 5 nominal concentrations (0.18-1.8 mg/l) and laboratory water control.
Reference: EA, Japan (1992)

(b)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Guppy
Exposure period: 96 hr
Results: $LC_{50\ (24h)}$ = 1.37 mg/l
$LC_{50\ (48h)}$ =
$LC_{50\ (72h)}$ =
$LC_{50\ (96h)}$ = 1.37 mg/l
NOEC =
LOEC =
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile
Remarks: None
Reference: Henderson et al. (1961)

(c)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Fathead Minnow

Exposure period: 96 hr
Results: $LC_{50\ (24h)}$ = 0.9 mg/l
$LC_{50\ (48h)}$ =
$LC_{50\ (72h)}$ =
$LC_{50\ (96h)}$ = 0.9 mg/l
NOEC =
LOEC =
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile
Reference: Henderson et al. (1961)

(d)
Type of test: static [**]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Fathead Minnow
Exposure period: 96 hr
Results: $LC_{50\ (24h)}$ = 0.75 mg/l
$LC_{50\ (48h)}$ = 0.73 mg/l
$LC_{50\ (72h)}$ = 0.73 mg/l
$LC_{50\ (96h)}$ = 0.71 mg/l
NOEC =
LOEC =
Analytical monitoring:Yes **[ ]** No **[ ]** ? **[X]**
Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile
Remarks: None
Reference: Henderson et al. (1961)

(e)
Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Bluegill
Exposure period: 96 hr
Results: $LC_{50\ (24h)}$ = 0.9 mg/l
$LC_{50\ (48h)}$ =
$LC_{50\ (72h)}$ =
$LC_{50\ (96h)}$ = 0.9 mg/l
NOEC =
LOEC =
Analytical monitoring:Yes **[ ]** No **[ ]** ? **[X]**
Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile

Remarks: None
Reference: Henderson et al. (1961)

(f)
Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[ ]**; closed-system **[ ]**
Species: Carp
Exposure period: 94 hr
Results: $LC_{50\ (5h)}$ = 125 mg/l
$LC_{50\ (24h)}$ =
$LC_{50\ (48h)}$ =
$LC_{50\ (72h)}$ =
$LC_{50\ (94h)}$ = 79-89 mg/l
$LC_{50\ (96h)}$ =
NOEC =
LOEC =
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile
Remarks: None
Reference: Loeb, H.A. & Kelly, W.H. (1963)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

A. Daphnia

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**;
open-system **[**X**]**; closed-system **[ ]**
Species: *Daphnia magna*
Exposure period: 24 hr
Results: $EC_{50\ (24h)}$ = 17 mg/l (95% confidence level: 13-21 mg/l)
$EC_{50\ (48h)}$ =
NOEC =
LOEC =
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD Test Guideline 202 (1984)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: 2-Hydroxypropanenitrile, purity: = 92.3 %
Remarks: 20 daphnids (4 replicates; 5 organisms per replicate) were exposed to 5 nominal concentrations (10-100 mg/l) and laboratory water control.
Reference: EA, Japan (1992)

B. Other aquatic organisms

No studies located

4.3 TOXICITY TO AQUATIC PLANTS e.g. Algae

Species:	*Selenastrum capricornutum* ATCC 22662
End-point:	Biomass **[X]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:	72 hours
Results:	Biomass: $EC_{50\ (24h)}$ =
	$EC_{50\ (72h)}$ = 0.14 mg/l
	NOEC = < 0.048 mg/l ($p < 0.05$)
	LOEC =
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	open-system **[**X**]**; closed-system **[ ]**
	OECD Test Guideline 201 (1984)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	2-Hydroxypropanenitrile, purity = 92.3 %
Remarks:	The EC_{50} values were calculated based on 5 nominal concentrations (0.05-0.50 mg/l)
Reference:	EA, Japan (1992)

4.4 TOXICITY TO BACTERIA

No studies located

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1. CHRONIC TOXICITY TO FISH

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species:	Fathead Minnow
End-point:	Length of young fish **[ ]**; Weight of young fish **[ ]**; Reproduction rate **[ ]**; Other **[ ]**
Exposure period:	20 days
Results:	
Mortality:	$LC_{50\ (..d)}$ =
	$LC_{50\ (20d)}$ = 0.69 mg/l
	NOEC =
	LOEC =
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**

Method:
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile, purity: unknown
Remarks: None
Reference: Henderson et al. (1961)

4.5.2. CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

(a)
Type of test: static **[ ]**; semi-static **[**X**]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna*
End-point: Mortality **[X]**; Reproduction rate **[X]**; Other **[ ]**
Exposure period: 21 day
Results:
Mortality: $LC_{50\ (24\ h)}$ = 4.8 mg/l (95% confidence level: 2.8-11 mg/l)
$LC_{50\ (48\ h)}$ = 2.5 mg/l (95% confidence level: 1.6-4.8 mg/l)
$LC_{50\ (96\ h)}$ = 1.9 mg/l (95% confidence level: 1.3-3.1 mg/l)
$LC_{50\ (7\ d)}$ = 1.4 mg/l (95% confidence level: 0.96-2.1 mg/l)
$LC_{50\ (14\ d)}$ = 0.84mg/l (95% confidence level: 0.62-1.2 mg/l)
$LC_{50\ (21\ d)}$ = 0.71mg/l (95% confidence level: 0.52-0.98 mg/l)
NOEC =
LOEC =
Reproduction: $EC_{50\ (14\ d)}$ = 0.78mg/l (95% confidence level: 0.5-1.2 mg/l)
$EC_{50\ (21\ d)}$ = 0.67mg/l (95% confidence level: 0.49-0.93 mg/l)
NOEC = 0.17mg/l ($p < 0.05$)
LOEC = 0.56mg/l ($p < 0.05$)
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD Test Guideline 202 (1984)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: 2-Hydroxypropanenitrile, purity = 92.3%
Remarks: 40 daphnids (4 replicates; 10 organisms per replicate) were exposed
to 5 nominal concentrations (0.056-5.6 mg/l) and laboratory water control.
Reference: EA, Japan (1992)

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

No studies located

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

No studies located

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

No studies located

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

No studies located

4.8 BIOTRANSFORMATION AND KINETICS IN ENVIRONMENTAL SPECIES

No studies located

4.9 ADDITIONAL REMARKS

None

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 (SD/Crj:CD)
Value :	31.0 (mg/kg) for male
	41.1 (mg/kg) for female
Method:	OECD Tsdt guideline 401 (1987)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	2-Hydroxypropanenitrile, purity: 92.3 %
Remarks:	None
Reference:	MHW, Japan (1993a)

(b)

Type :	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Rat
Value :	87 (mg/kg)
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	2-Hydroxypropanenitrile, purity: unknown
Remarks:	None
Reference:	Amer. Ind. Hyg. Assoc. J. (1969)

5.1.2 ACUTE INHALATION TOXICITY

Type :	LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[X]**; Other **[ ]**
Species/strain:	Rat
Exposure time:	4 hours
Value:	124 ppm
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	2-Hydroxypropanenitrile, purity: unknown
Remarks:	None
Reference:	Amer. Ind. Hyg. Assoc. J. (1969)

5.1.3 ACUTE DERMAL TOXICITY

Type :	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Rabbit
Value:	20 (mg/kg b.w.)
Method:	Unknown

GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 2-Hydroxypropanenitrile, purity: unknown
Remarks: None
Reference: Amer. Ind. Hyg. Assoc. J. (1969)

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

No studies located

5.2 CORROSIVENESS/IRRITATION

No studies located

5.2.1 SKIN IRRITATION/CORROSION

No studies located

5.2.2 EYE IRRITATION/CORROSION

No studies located

5.3 SKIN SENSITISATION

No studies located

5.4 REPEATED DOSE TOXICITY

Species/strain: Rat (Crj:CD(SD))
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: oral gavage
Exposure period: Males: 43 days including 14 days before mating
Females: from 14 days before mating to day 3 of lactation
Frequency of treatment: 7 days/week
Post exposure observation period:
Dose: 0, 1.2, 6 or 30 mg/kg (10 animals /group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL: 6 mg/kg/day
LOEL: 30 mg/kg/day
Results: Transient hypolocomotion, hypopnea, and salivation were found in the 30 mg/kg groups of both sexes. There were no visible differences in body weight, food consumption, or hematological

parameters between the treated and control animals of both sexes. In an investigation of clinical chemistry parameters, a decrease in GOT and increase in total protein, albumin, and calcium were found in the 30 mg/kg group of males. Increased absolute and relative liver weights occurred in 30 mg/kg male group. In a pathological examination, enlargement of the liver was also observed in the 30 mg/kg group of males. This was revealed to be due to a centrilobular hypertrophy and a fatty change of hepatocytes in a histopathological examination.

Method: OECD Combined Repeat dose and Reproductive/Developmental Screening Toxicity Test (1992)
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Commercial, purity: 92.3 %
Reference: MHW, Japan (1993b)

5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

(a)
Type : Bacterial reverse mutation assay
System of testing:
Species/strain: *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 0, 4.69, 9.38, 18.75, 37.5, 75 or 150 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: 150 µg/plate
Without metabolic activation: 150 µg/plate
Precipitation conc:
Genotoxic effects:

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

Method: Japanese Guideline for Screening Mutagenicity testing of chemicals
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Teat substance: Commercial, purity: 92.3%
Remarks: Procedure: Plate method
Plates/test: 3
Activation system: Liver S-9 fraction from Phenobarbital and 5,6-Benzoflavone pretreated male SD rats with NADPH-generating
system
Media:Histidine selective
No. replicates: 2
Reference: MHW, Japan (1993c)

(b)

Type :	Bacterial reverse mutation assay
System of testing:	
Species/strain:	*E. coli* WP2 uvrA
Concentration:	0, 75, 150, 300, 600, 1200 or 2400 µg/plate
Metabolic activation:	With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:	
Cytotoxicity conc:	With metabolic activation: 2400 µg/plate Without metabolic activation: 2400 µg/plate
Precipitation conc:	
Genotoxic effects:	+ ? - With metabolic activation: **[ ] [ ] [X]** Without metabolic activation: **[ ] [ ] [X]**
Method:	Japanese Guideline for Screening Mutagenicity testing of chemicals
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Teat substance:	Commercial, purity: 92.3%
Remarks:	Procedure: Plate method Plates/test: 3 Activation system: Liver S-9 fraction from Phenobarbital and 5,6-Benzoflavone pretreated male SD rats with NADPH-generating system No. replicates: 2
Reference:	MHW, Japan (1993c)

B. NON-BACTERIAL IN VITRO TEST

Type :	Cytogenetics Assay
System of testing:	
Species/strain:	Chinese hamster CHL cells
Concentration:	Incubated with 0, 0.10, 0.19 or 0.38 mg/ml (-S9) 0, 0.18, 0.36 or 0.71 mg/ml (+S9)
Metabolic activation:	With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:	
Cytotoxicity conc:	With metabolic activation: 1.00 mg/ml Without metabolic activation: 0.38 mg/ml
Precipitation conc:	
Genotoxic effects:	+ ? - With metabolic activation: **[X] [ ] [ ]** Without metabolic activation: **[X] [ ] [ ]**
Method:	Japanese Guideline for Screening Mutagenicity testing of chemicals chemicals
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Commercial, purity 92.3 %

Remarks: Plates/test:2
Activation system: S-9 fraction from the liver of Phenobarbital and 5,6-Benzoflavone induced male SD derived rats with NADPH-generating system
Media: RPMI 1640 medium *plus* 10% foetal calf serum *plus* phytohaemagglutinin
No. replicates: 1
Reference: MHW, Japan (1993c)

5.6 GENETIC TOXICITY IN VIVO

No studies located

5.7 CARCINOGENICITY

No studies located

5.8 TOXICITY TO REPRODUCTION

Type: Fertility **[ ]**; One generation study **[ ]**; Two generation study **[ ]**; Other **[X]**

Species/strain: Rat slc:SD
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral, gavage
Exposure period: Males: 43 days including 14 days before mating
Females: from 14 days before mating to day 3 of lactation.
Frequency of treatment: 7 days/week
Postexposure observation period:
Premating exposure period: male: 14 days, female: 14 days
Duration of the test;
Doses: 0, 1.2, 6, or 30 mg/kg (10 /animals/sex/group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**;
Historical **[ ]**
NOEL Parental : 30 mg/kg/day
NOEL F1 Offspring: 30 mg/kg/day
NOEL F2 Offspring: N/A
Results: There were no effects on mating, fertility and oestrus cycle or on dams during the pregnancy and lactation period. External examination of pups revealed no increase in appearance of abnormal pups. Body weight gain of pups was normal. Pups killed at postnatal day 4 showed no abnormal gross findings.

	General parental toxicity: see section 5.4.
	For toxicity to offspring: None
Method:	OEECD Combined Repeated Dose and Reproductive toxicity test
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Commercial, purity 92.3 %
Remarks:	
Reference:	MHW, Japan (1993b)

5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

No studies located

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

No studies located

B. Toxicodynamics, toxicokinetics

No studies located

5.11 EXPERIENCE WITH HUMAN EXPOSURE

None

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