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2,2'AZOBIS(2-METHYLPROPIONITRILE)
CAS N°: 78-67-1

SIDS Initial Assessment Report

for

9th SIAM

(France, June 29-July 1, 1999)

Chemical Name: 2,2'-Azobis(2-methylpropionitrile)
CAS No: 78-67-1
Sponsor Country: Japan

National SIDS Contact Point in Sponsor Country:

Mr. Kazuhide Ishikawa
Ministry of Foreign Affairs, Japan

HISTORY:

SIDS Testing Plan were reviewed in SIDS Review Process, where the following SIDS Testing Plan was agreed:

no testing ()

testing (X) Water solubility, Vapour pressure, Octanol/water partition coefficient, Stability in water, Biodegradation

Chronic toxicity to daphnia

Combined repeat dose and reproductive toxicity,

Gene mutation, Chromosomal aberration test in vitro

Deadline for circulation: March 31, 1999

Date of Circulation: March 30, 1999

(To all National SIDS Contact Points and the OECD Secretariat)

SIDS INITIAL ASSESSMENT PROFILE

CAS NO.	78-67-1
CHEMICAL NAME	2,2'-Azobis(2-methylpropionitrile)
Structural formula	$(\text{H}_3\text{C})_2\text{C}(\text{CN}) \text{N}=\text{NC}(\text{CN})(\text{CH}_3)_2$

RECOMMENDATIONS OF THE SPONSOR COUNTRY

The chemical is currently of low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE RECOMMENDATIONS

2,2'-Azobis(2-methylpropionitrile) is not readily biodegradable (OECD 301C: 0% after 28-day), and it is stable in water ($T_{1/2} = 304$ days at pH 7).

72-h EC_{50} of algae, *Selenastrum capricornutum* is more than 9.4 mg/l, and 72h NOEC is 4.2 mg/l. For the *Daphnia magna* test, 48-h EC_{50} for immobilisation is more than 10 mg/l, and 21-day EC_{50} and 21-day NOEC for reproduction are 7.5 mg/l and 2.2 mg/l, respectively. For testing in fish, Medaka (*Oryzias latipes*), 96-h and 14-day LC_{50} values are both more than 10 mg/l. No data are available for effects on terrestrial organisms.

2,2'-Azobis(2-methylpropionitrile) is considered not to be irritating to skin and eyes, or a skin sensitizer. In an OECD combined repeat dose and reproductive/developmental toxicity study in rats at 2, 10 and 50 mg/kg/day, this chemical was toxic to the liver as well as the kidneys. Increases in eosinophilic bodies and basophilic changes of the renal tubular epithelial cells in the kidneys were observed only in treated male rats. This male rat specific renal toxicity might be caused by accumulation of $\alpha_2\text{u}$ -macroglobulin as one of the possible mechanisms. Centrilobular hypertrophy of hepatocytes with the related changes in hepatotoxic blood parameters was detected at the middle and high doses in both sexes. NOAEL for repeated dose toxicity was considered to be 2 mg/kg/day, based on hepatic toxicity. As there was only a reduction in viability and body weight of offsprings after birth at the high dose, most likely due to maternal toxicity, NOAEL for reproductive toxicity was considered to be 50 mg/kg/day. This chemical may not be genotoxic, based on negative results of bacterial mutation testing and chromosomal aberration *in vitro* testing.

The production volume of 2,2'-Azobis(2-methylpropionitrile) is 1,100 tons/year in 1993 in Japan. This chemical is used in closed systems as an initiator of polymerisation in polymer industry, and not included in consumer products, therefore no consumer exposure is expected.

This chemical is released into the environments from the production and process sites, and as an example its amount is reported to be 1 kg/year by a processor who treats 12 tonnes/year. A generic fugacity model (Mackey level III) shows that most (98.6%) of this chemical will distribute in water phase after it is discharged into water.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE

FULL SIDS SUMMARY

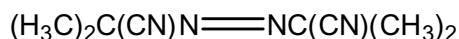
CAS NO: 78-67-1		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point			100 - 103 °C
2.2	Boiling Point			Decomposed
2.3	Density			
2.4	Vapour Pressure		OECD TG 104	0.810 Pa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	1.10
2.6 A.	Water Solubility		OECD TG 105	350 mg/l at 25 °C
B.	pH			
	pKa			
2.12	Oxidation: Reduction Potential			
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation			
3.1.2	Stability in Water		OECD TG 111	T _{1/2} = 263 day at pH4 at 25 °C T _{1/2} = 304 day at pH7 at 25 °C T _{1/2} = 210 day at pH9 at 25 °C
3.2	Monitoring Data			In air = not detected In surface water = not detected In soil/sediment = not detected
3.3	Transport and Distribution		Calculated (Fugacity Level III type)	Release: 100% to Water In Air 0.5 % In Water 98.6 % In Sediment 0.5 % In Soil 0.4 %
			(local exposure)	1.6 x 10 ⁻⁹ mg/L (Japan)
3.5	Biodegradation		OECD 301C	Not readily biodegradable 0% in 28 days
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	<i>Poecilia reticulata</i>	OECD TG 203	LD ₅₀ (96h) = > 10 mg/l LD ₅₀ (14d) = > 10 mg/l
4.2	Acute Toxicity to Aquatic Invertebrates <i>Daphnia</i>	<i>Daphnia magna</i>	OECD TG 202	EC ₅₀ (24hr) = > 10 mg/l EC ₅₀ (48hr) = > 10 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	<i>Selenastrum capricornutum</i>	ORCD TG 201	EC ₅₀ (72hr, Growth) = > 9.4 mg/l NOEC = 4.2 mg/l
4.5.2	Chronic Toxicity to Aquatic Invertebrates (<i>Daphnia</i>)	<i>Daphnia magna</i>	OECD TG 202	EC ₅₀ (21d, Repro) = 7.5 mg/l NOEC = 2.2 mg/l
4.6.1	Toxicity to Soil Dwelling Organisms			No Data
4.6.2	Toxicity to Terrestrial Plants			No Data
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)			No Data

TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	Other (unknown)	LD ₅₀ = 100 mg/kg b.w.
5.1.2	Acute Inhalation Toxicity	Rat	Other (unknown)	LC ₅₀ = > 12 g/m ³ /4 hr
5.1.3	Acute Dermal Toxicity			No data
5.2.1	Skin irritation/corrosion	Rabbit	OECD TG 404 and EC TG	No irritating
5.2.2	Eye irritation/corrosion	Rabbit	OECD TG 405 and EC TG	No irritating
5.3	Skin sensitisation	Guinea pig	OECD TG 406 and EC TG	No sensitizing
5.4	Repeated Dose Toxicity	Rat	OECD Combined	NOAEL = 2 mg/kg/day
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	<i>S. typhimurium</i> <i>E. coli</i> WP2	Japanese TG and OECD TG 471 & 472	- (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 combined	NOAEL = 50 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity			No data
5.11	Experience with Human Exposure			No data

[Note] Data beyond SIDS requirements can be added if the items are relevant to the assessment of the chemical, e.g. corrosiveness/irritation, carcinogenicity.

SIDS INITIAL ASSESSMENT REPORT**1. IDENTITY**

- OECD Name: 2,2'-Azobis(2-methylpropionitrile)
- Synonym: Azobisisobutyronitrile; Azodiisobutyrodinitrile; 2,2'-Azobis[2-methylpropanenitrile]; AIBN; alpha,alpha'-Azodiisobutyronitrile; 2,2'-Dicyano-2,2'-azopropane; Porofor-57; 2,2'-Azo-bis(isobutyronitrile); 2,2'-Dimethyl-2,2'-azodipropionitrile
- CAS Number: 78-67-1
- Empirical Formula: C₈H₁₂N₄
- Structural Formula:



- Degree of Purity: 99.3%
- Major Impurity: None
- Essential Additives: None
- Physical-chemical properties
 - Melting Point: 100 – 103 °C
 - Vapour pressure: 0.81 Pa at 25 °C
 - Water solubility: 350 mg/L
 - Log Pow: 1.10

2. GENERAL INFORMATION ON EXPOSURE**2.1 Production and import**

The production volume of 2,2'-azobis(2-methylpropionitrile) in Japan is 1,100 tonnes/year in 1995 and 12 tonnes are imported.

2.2 Use pattern

All of 2,2'-azobis(2-methylpropionitrile) produced and imported in Japan is used as a foaming agent for rubber and an initiator of polymerization, and no consumer uses are reported.

2.3 Other information

None

3. ENVIRONMENT**3.1 Environmental Exposure****3.1.1 General Discussion**

2,2'-Azobis(2-methylpropionitrile) is not biodegradable (OECD 301C: 0% after 28d) and stable in water ($T_{1/2} = 263,304$ and 210 day at pH 4,7,and 9, respectively). Although direct photodegradation

is expected because 2,2'-azobis(2-methylpropionitrile) has absorption band in UV and VIS region, the data of half-lifetime is not available.

2,2'-Azobis(2-methylpropionitrile) is low bioaccumulative based on Log Pow (1.10 at 25 °C).

The potential environmental distribution of 2,2'-azobis(2-methylpropionitrile) obtain from a generic Mackay level III fugacity model is shown in Table 1. Parameters used for this model are shown as Annex to this report. The results show that, if 2,2'-azobis(2-methylpropionitrile) is released into water, it is unlikely to be distributed into other compartment. If 2,2'-azobis(2-methylpropionitrile) is released into air or soil, it is likely to be distributed in water and soil.

Table 1
Environmental distribution of 2,2'-azobis(2-methylpropionitrile)
Using a generic level III fugacity model

Compartment	Release 100% to air	Release 100% to water	Release 100% to soil
Air	31.0 %	0.5 %	0.7 %
Water	40.9%	98.6 %	28.6 %
Soil	27.9 %	0.5 %	70.6 %
Sediment	0.2 %	0.4 %	0.1 %

As this chemical is used in closed system as an initiator of polymerization in polymer industry and is not included in consumer products, its release to the environment may occur only from the production site.

3.1.2 Predicted Environmental Concentration

As 2,2'-azobis(2-methylpropionitrile) is produced under the well controlled closed system, amount of release to air phase is negligibly small. The waste of 2,2'-azobis(2-methylpropionitrile) from the production system is released to water phase after treated its own wastewater treatment plant. Therefore, Predicted Environmental Concentration (PEC) will be calculated only for the water environment.

a) Regional exposure

According to report from a Japanese processor who import 12 t/y, 1kg/year (measured) of 2,2'-azobis(2-methylpropionitrile) are treated in its own wastewater treatment plant with 99.9% of removal rate (measured) and released with 6.24×10^8 L/year of effluent into sea. Local Predicted Environmental Concentration (PEC_{local}) is calculated to be 1.6×10^{-9} mg/L as a worst case scenario, employing the following calculation model and dilution factor of 1000(default).

$$\frac{\text{Amount of release (1 x 10}^6 \text{ mg/y) x (1 - Removal rate (99.9\%))}}{\text{Volume of effluent (6.24 x 10}^8 \text{ L/y) x Dilution Factor (1000)}}$$

3.2 Effects on the Environments

3.2.1 Effects on aquatic organisms

Acute and chronic toxicity data of 2,2'-azobis(2-methylpropionitrile) to aquatic organisms are summarized below (Table 2). Predicted no effect concentration (PNEC) of this chemical was

determined mainly based on the toxicity data obtained by the Environmental Agency of Japan through a GLP-laboratory.

As the lowest data among test organisms belonging to three trophic levels, 21d NOEC (2.2 mg/l) of *Daphnia magna* is selected. The assessment factor of 100 was adopted to chronic toxicity data to determine PNEC according to the OECD Provisional Guidance for Initial Assessment of Aquatic Effects (EXCH/MANUAL /96-4-5.DOC/May 1996), because chronic toxicity data for fish was absent.

From chronic toxicity data (NOEC of 21 d *Daphnia*):

$$\text{PNEC} = 2.2 / 100 = 0.022 \text{ mg/l}$$

Thus, PNEC of 2,2'-azobis(2-methylpropionitrile) is 0.022 mg/l.

The toxicity of 2,2'-azobis (2-methylpropionitrile) to test organisms is low. Any symptoms were not observed in the *Oryzias latipes* exposed to 9.6 mg/l (measured maximum concentration) in flow-through aquarium for 14-days.

Table 2
Toxicity data of 2,2'-azobis(2-methylpropionitrile) to aquatic organisms at different trophic levels. Relatively high toxicity data were selected from AQUIRE data base.

Species	Endpoint	Conc. (mg/l)	Remarks
Selenastrum capricornutum (algae)	Bms 72 h EC50	> 9.4	a, 1), A
	Bms 72 h NOEC	4.2	c, 1), C
<i>Daphnia magna</i> (Water flea)	Imm 48 h EC50	> 10	a, 1), A
	Rep 21 d EC50	7.5	c, 1)
	Rep 21d NOEC	2.2	c, 1), C
<i>Oryzias latipes</i> (fish, Medaka)	Mor 96 h LC50	>10	a, 1), A
	Mor 14 d LC50	>10	a, 1)

Notes: Bms; biomass, Imm; immobilization, Mor; mortality, Rep; reproduction, A), C); selected as the lowest value respectively among the acute or chronic toxicity data of algae, cladocera (water flea) and fishes to determine PNEC of 2,2'-azobis(2-methylpropionitrile). 1) Toxicity data were obtained by the Environment Agency of Japan based on OECD Test Guidelines and GLP.

3.2.2 Terrestrial effects

No available data

3.2.3 Other effects

No available data

3.3 Initial Assessment for the Environment

Predicted no effect Concentration (PNEC) of 2,2'-azobis(2-methylpropionitrile) for aquatic organisms is calculated based on the lowest acute and/or chronic toxicity data among algae, cladocera (water flea) and fishes and assessment factor of 100.

$$\text{PNEC} = 2.2 \text{ (NOEC of } Daphnia) / 100 = 0.022 \text{ mg/l}$$

The highest PEC from Japanese local exposure scenario is 1.6×10^{-9} mg/l

$$PEC_{\text{local}} / PNEC = 1.6 \times 10^{-9} / 0.022 = 7.3 \times 10^{-8} < 1$$

Thus, effects of this chemical on aquatic ecosystems are at low concern at present.

4. HUMAN HEALTH

4.1 Human Exposure

4.1.1 Occupational exposure

2,2'-Azobis(2-methylpropionitrile) is produced in closed systems and used as an initiator for polymer synthesis. The occupational exposure is expected through inhalation and dermal route is assumed negligible because this chemical is solid. As the atmospheric concentration in plant was not measured, the maximum exposure level is estimated according to working schedules as follows. If the worker (body weight; 70 kg, respiratory volume; 1.25 m³/hour) is assigned to implement this operation without protection, the highest daily intake (EHE) is calculated as 0.015 mg/kg/day as the worst case. Practically, the workers always wear protective gloves and respiratory protective equipment (mask) during the operation.

	Frequency Times/day	Duration hr	Working hr/day	Maximum Concentration mg/m ³	Maximum EHE mg/kg/day
Charging to Reaction Vessel	1	0.17	0.17	5.00	0.015

EHE: Estimated Human Exposure

4.1.2 Consumer exposure

All of 2,2'-azobis(2-methylpropionitrile) produced in Japan is used as an initiator of polymerization, and no consumer uses are reported in Sponsor country.

4.1.3 Indirect exposure via the environment

As 2,2'-azobis(2-methylpropionitrile) is persistent in water and low bioaccumulative, the exposure to the general population via the environment would be possible through drinking water processed from surface water.

The concentration in drinking water should be estimated to be equal to PEC calculated in Section 3.1, i.e. 1.6×10^{-9} mg/l. The daily intake through drinking water is calculated as 5.33×10^{-11} mg/kg/day (2 l/day, 60 kg b.w.).

Using the bioconcentration factor of 1.0 estimated from logPow, the concentration of this chemical in fish can be calculated as follows:

$$PEC_{\text{fish}} = (1.6 \times 10^{-9} \text{ mg/l}) \times 1.0 = 1.60 \times 10^{-12} \text{ mg/g-wet}$$

As a daily intake of fish in Japan is estimated to be 90 g for 60 kg body weight person, a daily intake of this chemical will be 2.40×10^{-12} mg/kg/day.

4.2 Effects on Human Health

a) Acute toxicity

[SIDS data] The oral LD₅₀ value for 2,2'-azobis(2-methylpropionitrile) was 100 mg/kg for rats. General anesthetic, somnolence, and ataxia were observed. In inhalation study, no mortality was observed at a concentration of 12 g/m³ for 4 hours. Exciting behavior, conjunctive irritation, and weight loss or decreased weight gain were observed (National Technical Information Service¹).

In another oral study, the LD₅₀ value was 700 mg/kg for mice (Merck Index: 1989).

The intraperitoneal LD₅₀ value was 25 mg/kg for rats (National Technical Information Service¹) and mice (National Technical Information Service²). General anesthetic, somnolence (general depressed activity), and ataxia were observed in rats.

The subcutaneous LD₀ values were 30, 40, 50, and 50 mg/kg for rats, mice, rabbits, and guinea pigs, respectively. Convulsions, effect on seizure threshold, and other changes in lungs, thorax, or respiration were observed in all species (*Archiv fuer Toxikologie*: 1957).

b) Irritation

In rabbit dermal study, 2,2'-azobis(2-methylpropionitrile) did not induce skin irritation at a single dose of 500 mg (Elf Atochem: 1996a).

Test in human also showed that this chemical was not a skin irritant (Kanerva *et al.*: 1997). The test was performed with 2 days occlusion and 3 readings (usually on day 2, 3 and 4-6). This chemical (0.1 %) was applied to 173 patients, suspected occupational dermatoses. Skin irritative reaction was observed only in one patient.

There was an eye irritation study, in which application of this chemical at a single dose of 100 mg into the conjunctival sac, induced no irritation approximately 1, 24, 48 and 72 hr after administration (Elf Atochem: 1996b).

Therefore, 2,2'-azobis(2-methylpropanitrile) is considered not to be a skin and eye irritant.

c) Sensitisation

It was showed that 2,2'-azobis(2-methylpropanitrile) was not a skin sensitizer by guinea pig maximization test (Elf Atochem: 1996c). In this study, intradermal injection of this chemical at 0.1 % and topical application at 500 mg were performed as an induction, and topical application of this chemical undiluted at 500 mg as challenge did not induce any response.

Allergic patch test in human also showed that this chemical was not a skin sensitizer (Kanerva *et al.*: 1997). This test was performed with 2 days occlusion and 3 readings (usually on day 2, 3 and 4-6). This chemical was applied at 1.0 % to 173 patients, who were suspected occupational dermatoses. No allergic reaction was observed.

Therefore, 2,2'-azobis(2-methylpropanitrile) is considered not to be a skin sensitizer.

d) Repeated toxicity

[SIDS data] Oral toxicity study was performed in SD (Crj: CD) rats by an OECD combined repeat dose and reproductive/developmental toxicity screening test. 2,2'-Azobis(2-methylpropanitrile) was administered by gavage at doses of 2, 10, 50 mg/kg for 45 days in males and from 14 days before mating to day 3 of lactation in females. (MHW, Japan: 1997)

In males, temporary salivation was induced in 10 mg/kg or more groups. Decrease in body weight gain and food consumption was observed at 50 mg/kg. In kidneys, absolute and relative weight was increased in all treatment group and in 10 mg/kg or more groups, respectively. In addition, increases in eosinophilic bodies and basophilic changes of the renal tubular epithelial cells were observed in all treatment groups and granular casts in the lower nephrons were observed in 10 mg/kg and more groups. Liver weights significantly increased by 14 and 66 % for absolute weight (14 and 74 % for relative weight) in 10 and 50 mg/kg group, respectively. Centrilobular hypertrophy of hepatocyte was observed in 10 and 50 mg/kg groups (\pm : 4 in 13, +: 9 in 13 for 10 mg/kg, ++: 13 in 13 for 50 mg/kg, compared to no changes in 0 and 2 mg/kg groups). In blood analysis conducted only in males, several changes were observed only in 50 mg/kg group.

In females, one female died on postpartum day 3 at 50 mg/kg. Decrease in body weight gain and food consumption was observed in 10 mg/kg and more groups. In kidneys, absolute and relative weight was increased at 50 mg/kg. Liver weights significantly increased by 43 % for absolute weight (51 % for relative weight) in only 50 mg/kg group. However, centrilobular hypertrophy of hepatocytes was observed in 10 and 50 mg/kg groups (\pm : 6 in 13, +: 1 in 13 for 10 mg/kg, \pm : 1 in 13, +: 11 in 13, ++: 1 in 13 for 50 mg/kg, compared to no changes in 0 and 2 mg/kg groups).

As renal pathological changes were observed only in males, accumulation of γ_2 -macroglobulin is suspected as a cause of male specific renal toxicity. Therefore, based on pathological changes in liver of both sexes, NOAEL was considered to be 2 mg/kg/day for both sexes.

e) Reproductive/developmental toxicity

Reproductive toxicity

[SIDS data] Oral toxicity study was performed in SD (Crj: CD) rats by an OECD combined repeat dose and reproductive/developmental toxicity screening test. 2,2'-Azobis(2-methylpropanitrile) was administered by gavage at doses of 2, 10, 50 mg/kg for 45 days in males and from 14 days before mating to day 3 of lactation in females. (MHW, Japan: 1997)

2,2'-Azobis(2-methylpropanitrile) showed no adverse effects on copulation, fertility, duration of pregnancy, gestation index and parturition at all treated groups. At 50 mg/kg (12 dams), three dams showed the difficulty of nursling and two of them let all their offsprings die within the first 4 days after birth. Although this chemical showed no adverse effects on viability, sex ratio and body weight of newborns at birth, viability and body weight of nurslings on postnatal day 4 at 50 mg/kg were lower than the control levels. These changes were considered to be caused by maternal toxicity. There were no morphological abnormalities in pups at all treated groups. Therefore, NOAEL for reproductive toxicity was considered to be 50 mg/kg/day.

f) Genetic toxicity

Bacterial test

[SIDS data] Gene reverse mutation was negative in *S. typhimurium* TA98, TA100, TA1535, TA1537, *E. coli* WP2 *uvrA* with and without metabolic activation, and TA97 without S9 mix. (MHW, Japan: 1997)

Non-bacterial test *in vitro*

[SIDS data] In chromosomal aberration test using cultured Chinese hamster lung (CHL/IU) cells, the negative result was obtained. (MHW, Japan: 1997)

In SOS chromotest, 2,2'-azobis(2-methylpropanitrile) showed borderline result in *E.coli* PQ37, but negative result in *E. coli* PM21 and GC4798. (Eder *et al.*: 1989)

Based on these results, 2,2'-azobis(2-methylpropanitrile) is considered not to be genotoxic.

4.3 Initial Assessment for Human Health

2,2'-Azobis(2-methylpropanitrile) is considered neither to be irritating to skin and eye nor a skin sensitizer. In an OECD combined repeat dose and reproductive/developmental toxicity study in rats at 2, 10 and 50 mg/kg/day, this chemical was toxic to the liver as well as the kidneys. Increases in eosinophilic bodies and basophilic changes of the renal tubular epithelial cells in the kidneys were observed only in treated male rats. This male rat specific renal toxicity might be caused by accumulation of α_{2u} -macroglobulin as one of the possible mechanisms. Centrilobular hypertrophy of hepatocytes with the related changes in hepatotoxic blood parameters was detected at the middle and high doses in both sexes. NOAEL for repeated dose toxicity was considered to be 2 mg/kg/day, based on hepatic toxicity. As there was only a reduction in viability and body weight of offsprings after birth at the high dose, most likely due to maternal toxicity, NOAEL for reproductive toxicity was considered to be 50 mg/kg/day. This chemical may not be genotoxic, based on negative results of bacterial mutation testing and chromosomal aberration *in vitro* testing.

Occupational exposure

2,2'-Azobis(2-methylpropanitrile) is imported and used as an initiator for polymer synthesis and workers wear protective gloves and respiratory protective equipment during the operation. Although the occupational exposure route may be an inhalation in limited workers, there is no available data of the atmosphere concentration. Based on the estimated concentration and the possibility of exposure period, the daily intake is calculated as 0.015 mg/kg/day as the worst case. As there is no toxicokinetics data, it is assumed that 100% absorption occurs across the lungs. Occupational risk is presumably low because the margin of safety is 133.

Consumer exposure

No consumer exposure is expected because of use pattern.

Indirect exposure via environment

As for indirect exposure via environment, PEC_{local} of 1.60×10^{-9} mg/l from local exposure scenario was used for the estimation. The daily intakes through drinking water and fish are calculated as 5.33×10^{-11} mg/kg/day and 2.40×10^{-12} mg/kg/day, respectively. Since the margin of safety is very large, such as 3.75×10^{10} for drinking water and 8.33×10^{11} for fish, health risk via environment is presumably low.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

2,2'-Azobis(2-methylpropionitrile) is not biodegradable (OECD 301: 0% after 28d) and stable in water ($T_{1/2} = 304$ days at pH 7). PEC/PNEC ratio is much less than 1 based on the local exposure scenario in the Sponsor country and PNEC, 0.022 mg/l (NOEC of *Daphnia magna*). It is currently considered of low potential risk for environments and low priority for further work.

2,2'-Azobis(2-methylpropionitrile) is toxic in a repeated dose study (i.e. liver, kidney), such as 2 mg/kg/day of NOAEL. In reproductive/developmental toxicity screening study, this chemical shows only maternal toxicity with the result of fetal toxicity (decrease in mortality and body weight gain). This chemical is neither irritating to the skin and eyes, nor a skin sensitizer. This chemical is not genotoxic. Occupational risk is expected to be low because margin of safety is calculated as 133. The margin of safety via indirect exposure is 3.75×10^{10} for drinking water and 8.33×10^{11} for fish, respectively. Therefore, it is currently considered of low potential human risk and low priority for further work.

5.2 Recommendations

No recommendation

6. REFERENCES

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- National Technical Information Service¹. (Springfield, VA 22161) OTS0555369
- National Technical Information Service². (Springfield, VA 22161) AD691-490

Appendix 1. Method for Prediction of Environmental Concentration of Pollutant in Surface Water

1. Predicted environmental concentration in the local environment (PEC_{local}) with effluent release into river

When decomposition, precipitation and vaporization of pollutant can be ignored, it is used that simplified equation by complete mixing model shown with equation (1) to calculate predicted environmental concentration in the local environment (PEC_{local}) as for release effluent into river.

$$\text{PEC}_{\text{local}} \text{ (mg/L)} = \frac{C_o Q + C_s Q_s}{Q + Q_s} \quad (1)$$

Where

C_o: Concentration of pollutant in upper stream of release point (mg/L)

C_s: Concentration of pollutant in effluent (mg/L)

Q: Flow rate of river (m³/day)

Q_s: Flow rate of effluent released into river (m³/ day)

At the equation (1), when C_o can be considered as 0, dilution factor of pollutant in the river (R) can be shown with following equation.

$$R = C_s/C = (Q + Q_s) / Q_s \quad (2)$$

As the worst case, it is used to employ a flow rate at dry season as flow rate of river (Q). When flow rate at dry season is indistinct, it is estimated using the following equation in Japan.

$$\text{Flow rate at dry season} = \text{mean flow late} / 2.5 \quad (3)$$

2. Predicted environmental concentration in the local environment (PEC_{local}) with effluent release into sea

For prediction of concentration of pollutant in the sea water with effluent, it is employed generally Joseph-Sendnersymbol 146 \f "Times New Roman" \s 11'}s equation (4). This equation is one of analytic solution led under the following conditions from diffusion equation.

- 1 It is adopted large area of sea or lake.
- 2 The flow rate of effluent and concentration of pollutant in the effluent are constant, and distribution of concentration is able to regard as equilibrium state.
- 3 Effluent is distributed uniformly to vertical direction, and it spreads in a semicircle or segment to horizontal direction.
- 4 Diffusion coefficient of pollutant at the sea is in proportion to distance from release point of effluent.
- 5 There is not any effect of tidal current.
- 6 Decomposition of pollutant can be ignored.

$$C(x) = (C_s - C(r)) \left(1 - \exp \left(- \frac{Q_s}{d p} \left(\frac{1}{x} - \frac{1}{r} \right) \right) \right) + C(r) \quad (4)$$

Where

$C(x)$: Concentration of pollutant at distance x (m) from release point

C_s : Concentration of pollutant in effluent

$C(r)$: Concentration of pollutant at distance r (m) from release point

Q_s : Flow rate of effluent (m^3/day)

θ : Opening angle of seacoast (rad.)

d : Thickness of diffusion layer (m)

P : Diffusion velocity (m/day) (1.0–0.5 cm/sec)

When $C(x)$ is 0 at $r = \infty$ and density stratification is ignored for simplification, Joseph-Sendner's equation (4) is simplified to equation (5)

$$C(x) = C_s \left(1 - \exp \left(- \frac{Q_s}{d p x} \right) \right) \quad (5)$$

Because of $Q_s / d p x \ll 1$ except vicinity of release point, dilution factor R in distance x from release point $R(x)$ can be shown with equation (6).

$$R(x) = C_s / C(x) = d p x / Q_s \quad (6)$$

When it is employed following parameters in equation (6) as default, dilution factor R can be shown with equation (7).

$$P = 1 \text{ cm/sec (860 m/day)}$$

$$= 3.14$$

$$d = 10 \text{ m}$$

$$x = 1000 \text{ m}$$

$$R = 2.7 \cdot 10^7 / Q_s \quad (7)$$

Q_s : volume of effluent (m^3/day)

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE 5 CHEMICAL
2,2'-Azobis(2-methylpropionitrile)

CAS No. 78-67-1

Sponsor Country: Japan

DATE: March 31, 1999

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Appendix 1

Note: *; Data elements in the SIDS

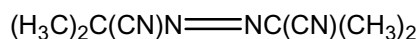
†; Data elements specially required for inorganic chemicals

SIDS PROFILE

1.01 A.	CAS No.	78-67-1
1.01 C.	CHEMICAL NAME (OECD Name)	2,2'-Azobis(2-methylpropionitrile)
1.01 D.	CAS DESCRIPTOR	
1.01 G.	STRUCTURAL FORMULA	$(\text{H}_3\text{C})_2\text{C}(\text{CN})\text{N}=\text{NC}(\text{CN})(\text{CH}_3)_2$
	OTHER CHEMICAL IDENTITY INFORMATION	
1.5	QUANTITY	Production: 1,100 tonnes/year Import volume: 12 tonnes/year in Japan
1.7	USE PATTERN	Intermediate Intermediate in closed system. Initiator for polymerization.
1.9	SOURCES AND LEVELS OF EXPOSURE	1 kg/year Release into river
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)	SIDS testing required: Water solubility, Vapour pressure, Octanol/water partition coefficient, Stability in water, Biodegradation Chronic toxicity to daphnia, Combined repeat dose and reproductive toxicity, Gene mutation, Chromosomal aberration test in vitro	

SIDS SUMMARY

CAS NO: 78-67-1		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	N						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
2.12	Oxidation: Reduction potential	N						N
OTHER P/C STUDIES RECEIVED								
ENVIRONMENTAL FATE and PATHWAY								
3.1.1	Photodegradation	N						N
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
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	N						N
5.4	Repeated Dose	N						Y
5.5	Genetic Toxicity <i>in vitro</i>							
	. Gene mutation	N						Y
	. Chromosomal aberration	N						Y
5.6	Genetic Toxicity <i>in vivo</i>	N						N
5.8	Reproduction Toxicity	N						Y
5.9	Development / Teratogenicity	N						N
5.11	Human experience	N						N
OTHER TOXICITY STUDIES RECEIVED								

1. GENERAL INFORMATION**1.01 SUBSTANCE INFORMATION*****A. CAS number** 78-67-1**B. Name (IUPAC name)*****C. Name (OECD name)** 2,2'-Azobis(2-methylpropionitrile)**†D. CAS Descriptor****E. EINECS-Number** 201-132-3**F. Molecular Formula** C₈H₁₂N₄***G. Structural Formula****H. Substance Group****I. Substance Remark****J. Molecular Weight** 164.21**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)
 Environmental Agency (EA)
 Ministry of Labour (MOL)

Contact person: Mr. Kazuhide Ishikawa
 Economic International Bureau
 Second International Organization Division
 Ministry of Foreign Affairs

.....
 2-2-1 Kasumigaseki, Chiyoda-ku, Tokyo 100 Japan
 Tel: 81-3-3581-0018
 Fax: 81-3-3503-3136

C. Name of responder

Same as above contact person

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance element []; inorganic []; natural substance []; organic [X]; organometallic []; petroleum product []

B. Physical State (at 20°C and 1.013 hPa)

gaseous []; liquid []; solid [X]

C. Purity

1.2 SYNONYMS

Azobisisobutyronitrile; Azodiisobutyrodinitrile; 2,2'-Azobis[2-methylpropanenitrile]; AIBN; alpha,alpha'-Azodiisobutyronitrile; 2,2'-Dicyano-2,2'-azopropane; Porofofor-57; 2,2'-Azobis(isobutyronitrile); 2,2'-Dimethyl-2,2'-azodipropionitrile

1.3 IMPURITIES

None

1.4 ADDITIVES

None

***1.5 QUANTITY**

Remarks: 1,100 tonnes/year

Reference: MITI, Japan

1.6 LABELLING AND CLASSIFICATION

None

***1.7 USE PATTERN**

A. General

Type of Use:**Category:**

main	Intermediate
industrial	Intermediate in closed system
use	Initiator for polimerization

Remarks: None

Reference: MITI, Japan

1.8 OCCUPATIONAL EXPOSURE LIMIT

None

*** 1.9 SOURCES OF EXPOSURE**

In Japan, 2,2'-azobis(2-methylpropionitrile) is produced in 2 companies.

Source: Media of release: River
Quantities per media: 1 kg/year (one company)
Remarks:
Reference: MITI, Japan

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: 100 - 103 °C
Decomposition: Yes [] No [X] Ambiguous []
Sublimation: Yes [] No [X] Ambiguous []
Method:
GLP: Yes [] No [X] ? []
Remarks:
Reference: MITI, Japan

*2.2 BOILING POINT

Value: decompose
Pressure:
Decomposition: Yes [X] No [] Ambiguous []
Method:
GLP: Yes [] No [X] ? []
Remarks:
Reference:

*2.4 VAPOUR PRESSURE

Value: 8.1×10^{-1} Pa
Temperature: 25 °C
Method: calculated []; measured [X]
OECD TG 104
GLP: Yes [X] No [] ? []
Test substance: purity: 99.6 %
Remarks:
Reference: MITI, Japan

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

Log Pow: 1.10
Temperature: 25 °C
Method: calculated []; measured [X]
OECD TG 107
GLP: Yes [X] No [] ? []
Test substance: purity: 98 %
Remarks:
Reference: MITI, Japan

2.6 WATER SOLUBILITY*A. Solubility**

Value: 350 mg/L
 Temperature: 25 °C
 Description: Miscible []; Of very high solubility []; Soluble []; Slightly soluble [X]; Of low solubility []; Of very low solubility []; Not soluble []
 Method: OECD TG 105
 GLP: Yes [X] No [] ? []
 Test substance: purity: 99.6 %
 Remarks:
 Reference: MITI, Japan

B. pH Value, pKa Value

No ionizable Functional Group

3. ENVIRONMENTAL FATE AND PATHWAYS**3.1 STABILITY*****3.1.2 STABILITY IN WATER**

Type: Abiotic (hydrolysis) [X]; biotic (sediment)[]
 Half life: 263 days at pH 4 at 25 °C
 304 days at pH 7 at 25 °C
 210 days at pH 9 at 25 °C
 Method: OECD TG 111
 GLP: Yes [X] No [] ? []
 Test substance: purity: 99.6 %
 Remarks:
 Reference: MITI, Japan

***3.2 MONITORING DATA (ENVIRONMENTAL)**

- (a) Type of Measurement: Background []; At contaminated site []; Other [X]
 Media: Surface water (river)
 Results: ND (Detection limits: 0.01 mg/l) in 1 area in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)
- (b) Type of Measurement: Background []; At contaminated site []; Other [X]
 Media: Surface water (estuary)
 Results: ND (Detection limits: 0.01 mg/l) in 1 area in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)
- (c) Type of Measurement: Background []; At contaminated site []; Other [X]

- Media: Surface water (sea)
 Results: ND (Detection limits: 0.01 mg/l) in 3 areas in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)
- (d) Type of Measurement: Background []; At contaminated site []; Other [X]
 Media: Sediment (river)
 Results: ND (Detection limits: 0.1 mg/kg-dry) in 1 area in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)
- (e) Type of Measurement: Background []; At contaminated site []; Other [X]
 Media: Sediment (estuary)
 Results: ND (Detection limits: 0.1 mg/kg-dry) in 1 area in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)
- (f) Type of Measurement: Background []; At contaminated site []; Other [X]
 Media: Sediment (sea)
 Results: ND (Detection limit: 0.1 mg/kg-dry) in 3 areas in Japan as of 1979
 Remarks: ND: Not detected
 Reference: Chemicals in the environment, EA, Japan (1980)

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

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

- Media: Air-biota []; Air-biota-sediment-soil-water [X]; Soil-biota []; Water-air []; Water-biota []; Water-soil []; Other []
 Method: Fugacity level I []; Fugacity level II []; Fugacity level III [X]; Fugacity level IV []; Other (calculation) []; Other (measurement)[]
 Results:

Compartment	Release 100% to air	Release 100% to water	Release 100% to soil
Air	31.0 %	0.5 %	0.7 %
Water	40.9 %	98.6 %	28.6 %
Soil	27.9 %	0.5 %	70.6 %
Sediment	0.2 %	0.4 %	0.1 %

- Remarks: Appendix 1
 Reference: MITI, Japan

*3.5 BIODEGRADATION

Type: aerobic ; anaerobic
 Inoculum: adapted ; non-adapted
 Concentration of the chemical: related to COD ; DOC ; test substance
 Medium: water ; water-sediment ; soil ; sewage treatment
 Degradation: 0 % by BOD after 28 days
 3 % by TOC after 28 days
 7 % by HPLC after 28 days
 Results: readily biodeg. ; inherently biodeg. ; under test condition
 no biodegradation observed , other
 Method: OECD TG 301C
 GLP: Yes No ?
 Test substance: purity: 99 %
 Reference: MITI, Japan

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

(a) Type of test: static ; semi-static ; flow-through ; other (*e.g. field test*)
 open-system ; closed-system
 Species: *Oryzias latipes* (Himedaka)
 Exposure period: 96 h
 Results: LC₅₀ (96 h) > 10 mg/l
 Analytical monitoring: Yes No ?
 Method: OECD TG 203 (1992)
 GLP: Yes No ?
 Test substance: As prescribed by 1.1 - 1.4, purity: 99.3 %
 Remarks: Groups of ten Himedaka were exposed to the nominal concentrations of 1.0, 1.8, 3.2, 5.6 and 10* mg/l, a solubilizer control (100 mg/l of DMF) and laboratory water control. The LC₅₀ (96h) was determined to be over 10 mg/l. 10* mg/l; the highest concentration dispersed completely by the maximum concentration of solubilizer (100 mg/l). Measured concentration was almost same as nominal concentration.
 Reference: Environment Agency of Japan (1996)

(b) Type of test: static ; semi-static ; flow-through ; other (*e.g. field test*)
 open-system ; closed-system
 Species: *Poecilia reticulata* (Guppy)
 Exposure period: 14 d
 Results: LC₅₀ (14d) > 10 mg/l
 Analytical monitoring: Yes No ?
 Method: OECD TG 203 (1992)
 GLP: Yes No ?
 Test substance: As prescribed by 1.1 - 1.4, purity: 99.3 %
 Remarks: Groups of ten Himedaka were exposed to the nominal concentrations of 1.0, 1.8, 3.2, 5.6 and 10* mg/l, a solubilizer control (100 mg/l of DMF) and laboratory water control. The LC₅₀ (14 d) was determined to be over 10 mg/l.

10* mg/l; the highest concentration dispersed completely by the maximum concentration of solubilizer (100 mg/l). Measured concentrations were almost same as nominal concentrations throughout the test period.

Reference: Environment Agency of Japan (1996)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test: static ; semi-static ; flow-through ; other (*e.g. field test*) ; open-system ; closed-system

Species: *Daphnia Magna*.

Exposure period: 48 h.

Results: EC₅₀ (48 h) > 10 mg/l

Analytical monitoring: Yes No ?

Method: OECD TG 202

GLP: Yes No ?

Test substance: As prescribed by 1.1 - 1.4, purity: 99.3 %

Remarks: 20 daphnids (4 replicates by 5 organisms) were exposed to the nominal concentrations of 10* mg/l, solubilizer control (DMF of 100 mg/l) and laboratory water control. 10* mg/l; the highest concentration dispersed completely by the maximum concentration of solubilizer (100 mg/l).

Reference: Environment Agency of Japan (1995).

Type of test: static ; semi-static ; flow-through ; other (*e.g. field test*) ; open-system ; closed-system

Species: *Daphnia Magna*.

Exposure period: 48 h.

Results: EC₅₀ (48 h) > 367 mg/l

Analytical monitoring: Yes No ?

Method: C2 of the European Directive 92/69/CEE

GLP: Yes No ?

Test substance: As prescribed by 1.1 - 1.4, purity: Unknown

Remarks: Since AZDN is sparingly soluble, the test was carried out with concentrations up to the water solubility. Daphnia were exposed in a static test to a concentration range of 160 to 367 mg/l, forming a geometric progression with a factor of 1.15. The test was performed with 20 daphnia per concentration. The test was performed using closed flasks as test glassware. The flasks were entirely filled with test solution and closed with butyl rubber caps covered with PTFE.

Reference: Service Analyse Environment (France)

*4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

Species: *Selenastrum capricornutum* ATCC 22662

Endpoint: Biomass ; Growth rate ; Other

Exposure period: 72 h

Results: Biomass EC₅₀ (72h) > 9.4 mg/l

	(Endpoint)	NOEC = 4.2 mg/l
Analytical monitoring:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Method:	OECD TG 201 (1984) open-system <input checked="" type="checkbox"/> ; closed-system <input type="checkbox"/>	
GLP:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.3 %	
Remarks:	Static test. The EC ₅₀ value for growth rate (% inhibition) was calculated based on 5 measured concentrations (0.46, 0.71, 2.1, 4.2 and 9.4 mg/l). DMF of 100 mg/l was used as a solubilizer.	
Reference:	Environment Agency of Japan (1996)	
Species:	<i>Pseudokirchneriella subcapitata</i> (<i>Selenastrum capricornutum</i>)	
Endpoint:	Biomass <input checked="" type="checkbox"/> ; Growth rate <input type="checkbox"/> ; Other <input type="checkbox"/>	
Exposure period:	72 h	
Results:	Biomass	EC ₅₀ (72h) 2.9 mg/l NOEC = 2.2 mg/l
	Growth rate	EC ₅₀ (72h) 6.1 mg/l NOEC = 2.2 mg/l
Analytical monitoring:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Method:	OECD TG 201 (1984) open-system <input checked="" type="checkbox"/> ; closed-system <input type="checkbox"/>	
GLP:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Test substance:	As prescribed by 1.1 - 1.4, purity: Unknown	
Remarks:		
Reference:	Service Analyse Environment (France)	

4.4 TOXICITY TO BACTERIA

No data

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

No data

(* 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test:	static <input type="checkbox"/> ; semi-static <input checked="" type="checkbox"/> ; flow-through <input type="checkbox"/> ; other (<i>e.g. field test</i>) <input type="checkbox"/>]; open-system <input type="checkbox"/> ; closed-system <input checked="" type="checkbox"/>	
Species:	<i>Daphnia Magna</i> .	
Endpoint:	Mortality <input type="checkbox"/> ; Reproduction rate <input checked="" type="checkbox"/> ; Other <input checked="" type="checkbox"/>	
Exposure period:	21 d	
Results:	Reproduction rate:	EC ₅₀ (21 d) = 7.5 mg/l (Endpoint) NOEC = 2.2 mg/l LOEC = 4.6 mg/l
Analytical monitoring:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Method:	OECD TG 202(1984)	
GLP:	Yes <input checked="" type="checkbox"/> No <input type="checkbox"/> ? <input type="checkbox"/>	
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.3 %	

Remarks: 40 daphnids (4 replicate of 10 daphnids) were exposed to 5 nominal concentrations (0.46, 1.0, 2.2, 4.6, and 10 mg/l), solvent control (100 mg/l of acetone) control and laboratory water control (dechlorinated tap water, pH: 7.4 to 8.0; DO: 7.5 to 8.0 mg/l). Measured concentrations were within 88 to 98 % of the nominal concentrations throughout the 21-d test period.

Reference: Environment Agency of Japan (1995).

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

No data

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

No data

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

No data

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

No data

4.8 BIOTRANSFORMATION AND KINETICS

No data

4.9 ADDITIONAL REMARKS

None

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type: LD₀ []; LD₁₀₀ []; LD₅₀ [X]; LDL₀ []; Other []

Species/strain: Rats

Value: 100 mg/kg b.w.

Method: Other

GLP: Yes [] No [X] ? []

Test substance: purity: unknown

Remarks: General anesthetic, somnolence, and ataxia

Reference: National Technical Information Service¹

Type: LD₀ []; LD₁₀₀ []; LD₅₀ [X]; LD_{L0} []; Other []
 Species/strain: Mice
 Value: 700 mg/kg b.w.
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks:
 Reference: Merck Index: 1989

5.1.2 ACUTE INHALATION TOXICITY

Type: LC₀ []; LC₁₀₀ []; LC₅₀ []; LCL₀ [X]; Other []
 Species/strain: Rats
 Exposure time: 4 hr
 Value: > 12 g/m³
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: Exciting behavior, conjunctive irritation, weight loss or decreased weight gain
 Reference: National Technical Information Service¹

5.1.3 ACUTE DERMAL TOXICITY

No data

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

(a) Type: LD₀ []; LD₁₀₀ []; LD₅₀ [X]; LD_{L0} []; Other []
 Species/strain: Rats
 Route of Administration: i.m. []; i.p. [X]; i.v. []; infusion []; s.c. []; other []
 Exposure time:
 Value: 25 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: General anesthetic, somnolence (general depressed activity), and ataxia
 Reference: National Technical Information Service¹

(b) Type: LD₀ []; LD₁₀₀ []; LD₅₀ [X]; LD_{L0} []; Other []
 Species/strain: Mice
 Route of Administration: i.m. []; i.p. [X]; i.v. []; infusion []; s.c. []; other []
 Exposure time:
 Value: 25 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks:
 Reference: National Technical Information Service²

- (c) Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LD_{L0} [X]; Other []
 Species/strain: Rats
 Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. [X]; other []
 Exposure time:
 Value: 30 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: Convulsions or effect on seizure threshold, and other changes in lungs, thorax, or respiration
 Reference: *Archiv fuer Toxikologie: 1957*
- (d) Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LD_{L0} [X]; Other []
 Species/strain: Mice
 Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. [X]; other []
 Exposure time:
 Value: 40 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: Convulsions or effect on seizure threshold, and other changes in lungs, thorax, or respiration
 Reference: *Archiv fuer Toxikologie: 1957*
- (e) Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LD_{L0} [X]; Other []
 Species/strain: Rabbits
 Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. [X]; other []
 Exposure time:
 Value: 50 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: Convulsions or effect on seizure threshold, and other changes in lungs, thorax, or respiration
 Reference: *Archiv fuer Toxikologie: 1957*
- (f) Type: LD₀ []; LD₁₀₀ []; LD₅₀ []; LD_{L0} [X]; Other []
 Species/strain: Guinea pigs
 Route of Administration: i.m. []; i.p. []; i.v. []; infusion []; s.c. [X]; other []
 Exposure time:
 Value: 50 mg/kg
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: Convulsions or effect on seizure threshold, and other changes in lungs, thorax, or respiration
 Reference: *Archiv fuer Toxikologie: 1957*

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain:	New Zealand White rabbits
Results:	Highly corrosive []; Corrosive []; Highly irritating []; Irritating []; Moderate irritating []; Slightly irritating []; Not irritating [X]
Classification:	Highly corrosive (causes severe burns)[]; Corrosive (causes burns)[]; Irritating []; Not irritating []
Method:	OECD TG 404 and EC TG 92/69/E.E.C., B ₄
GLP:	Yes [X] No [] ? []
Test substance:	purity: 99.2 %
Remarks:	A single dose of 500 mg in original form of 2,2'-azobis(2-methylpropanitrile) was applied to the closely-clipped skin of the flank for 4 hours, with semi-occlusive dressing. Cutaneous reaction was evaluated approximately one hour, 24, 48 and 72 hours after removal of the dressing.
Reference:	Elf Atochem: 1996a
Species/strain:	Human
Results:	Highly corrosive []; Corrosive []; Highly irritating []; Irritating []; Moderate irritating []; Slightly irritating []; Not irritating [X]
Classification:	Highly corrosive (causes severe burns)[]; Corrosive (causes burns)[]; Irritating []; Not irritating []
Method:	Other
GLP:	Yes [] No [X] ? []
Test substance:	purity: unknown
Remarks:	Test was performed with 2 days occlusion and 3 readings (usually on irritant day 2, 3 and 4-6). 1.0 % in petroleum ether was applied to 173 patients, who were suspected occupational dermatoses.
Reference:	Kanerva <i>et al.</i> : 1997

5.2.2 EYE IRRITATION/CORROSION

Species/strain:	New Zealand White rabbits
Results:	Highly corrosive []; Corrosive []; Highly irritating []; Irritating []; Moderate irritating []; Slightly irritating []; Not irritating [X]
Classification:	Irritating []; Not irritating []; Risk of serious damage to eyes []
Method:	OECD TG 405 and EC TG 92/69/E.E.C., B ₅
GLP:	Yes [X] No [] ? []
Test substance:	purity: 99.2 %
Remarks:	After gently pulling the lower lid away from the eyeball, a single dose of 100 mg in original form of 2,2'-azobis(2-methylpropanitrile) was administered into the conjunctival sac of the left eye. The lower and upper eyelids were held together for about one second to avoid any loss of test substance. The right eye, which remained untreated, served as a control. The eyes were not rinsed and examined approximately one hour, 24, 48 and 72 hours after administration.
Reference:	Elf Atochem: 1996b

5.3 SKIN SENSITISATION

Type: Maximization test
 Species/strain: Dunkin-Hartley guinea pigs
 Results: Sensitizing []; Not sensitizing [X]; Ambiguous []
 Classification: Sensitizing []; Not sensitizing []
 Method: OECD Guideline No. 406 and EC Guideline 92/69/E.E.C., B₆
 GLP: Yes [X] No [] ? []
 Test substance: purity: 99.2 %
 Remarks: On day 1, 0.1 % in paraffin oil or the vehicle was injected intradermally in the dorsal region between the shoulders. On day 7, the same region received a topical application of sodium lauryl sulfate in vaseline in order to induce local irritation. On day 8, topical application of undiluted substance (500 mg) or the vehicle to this same site was performed with an occlusive dressing for 48 hours. After rest period of 12 days, all animals were challenged by a topical application of undiluted substance (500 mg) and the vehicle to the right and the left flank, respectively. This application was held for 24 hours with an occlusive, hypoallergenic dressing. Skin reaction was evaluated approximately 24 and 48 hours after challenge application.
 Reference: Elf Atochem: 1996c

Type: Allergic and irritant patch test
 Species/strain: Human
 Results: Sensitizing []; Not sensitizing [X]; Ambiguous []
 Classification: Sensitizing []; Not sensitizing []
 Method: Other
 GLP: Yes [] No [X] ? []
 Test substance: purity: unknown
 Remarks: This test was performed with 2 days occlusion and 3 readings (usually on day 2, 3 and 4-6). 1.0 % in petroleum ether was applied to 173 patients, who were suspected occupational dermatoses.
 Reference: Kanerva *et al.*: 1997

***5.4 REPEATED DOSE TOXICITY**

Species/strain: Rats/Crj: CD (SD)
 Sex: Female []; Male []; Male/Female [X]; No data []
 Route of Administration: Oral (by gavage)
 Exposure period: Male: 42 days
 Female: From 14 days before mating to day 3 of lactation
 Frequency of treatment: Daily
 Post exposure observation period:
 Dose: 0, 2, 10, 50 mg/kg/day
 Control group: Yes [X]; No []; No data []; Corn oil
 Concurrent no treatment []; Concurrent vehicle [X]; Historical []
 NOAEL: Male: 2 mg/kg/day, Female: 2 mg/kg/day
 LOAEL: Male: 10 mg/kg/day, Female: 10 mg/kg/day

Results:	Male:	Temporary salivation was induced at 10 mg/kg or more groups. Decrease in body weight gain and food consumption was observed at 50 mg/kg. In kidneys, absolute and relative weight was increased in all treatment group and in 10 mg/kg or more groups, respectively. In addition, increases in eosinophilic bodies and basophilic changes of the renal tubular epithelial cells were observed in all treatment groups and granular casts in the lower nephrons were observed in 10 mg/kg and more groups. As these pathological changes were observed only in males, accumulation of α_{2u} -macroglobulin is suspected as a cause of male specific renal toxicity. Liver weights significantly increased by 14 and 66 % for absolute weight (14 and 74 % for relative weight) in 10 and 50 mg/kg group, respectively. Centrilobular hypertrophy of hepatocyte was observed in 10 and 50 mg/kg groups (\pm : 4 in 13, +: 9 in 13 for 10 mg/kg, ++: 13 in 13 for 50 mg/kg, compared to no changes in 0 and 2 mg/kg groups). In blood analysis, there were several changes in 50 mg/kg group, such as an elevation of platelet and white blood cell counts, increases in total protein, albumin, total cholesterol, Ca and inorganic phosphorus, and decreases in the A/G ratio and Cl concentration.
	Female:	One animal died on postpartum day 3 at 50 mg/kg. Decrease in body weight gain and food consumption was observed in 10 mg/kg and more groups. In kidneys, absolute and relative weights were increased at 50 mg/kg. Liver weights significantly increased by 43 % for absolute weight (51 % for relative weight) in only 50 mg/kg group. However, centrilobular hypertrophy of hepatocytes was observed in 10 and 50 mg/kg groups (\pm : 6 in 13, +: 1 in 13 for 10 mg/kg, \pm : 1 in 13, +: 11 in 13, ++: 1 in 13 for 50 mg/kg, compared to no changes in 0 and 2 mg/kg groups).
Method:		OECD Combined Repeat Dose and eproductive/Developmental Toxicity Screening Test
GLP:		Yes [X] No [] ? []
Test substance:		purity: 99.9 %
Reference:		MHW, Japan (1997)

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type:	Gene mutation test
System of testing:	<i>Salmonella typhimurium</i> TA98, TA100, TA1535, TA1537, TA97 (without S9 mix), <i>Escherichia coli</i> WP2 <i>uvrA</i>
Concentration:	+S9 mix; 0, 313, 625, 1250, 2500, 5000 μ g/plate (TA98, TA100, TA1535, TA1537, and WP2 <i>uvrA</i>) -S9 mix; 0, 313, 625, 1250, 2500, 5000 μ g/plate (all strains)
Metabolic activation:	With []; Without []; With and Without [X]; No data []
S9:	Rat liver, induced with phenobarbital and 5,6-benzoflavone
Results:	
Cytotoxicity conc:	With metabolic activation: Not observed

	Without metabolic activation: Not observed
Precipitation conc:	With metabolic activation: 1250 µg/plate
	Without metabolic activation: 2500 µg/plate
Genotoxic effects:	+ ? -
	With metabolic activation: [] [] [X]
	Without metabolic activation: [] [] [X]
Method:	Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD Guideline No. 471 and 472
GLP:	Yes [X] No [] ? []
Test substance:	purity: 99.9 %
Remarks:	Positive control: With metabolic activation: 2-Aminoanthracene (five strains) Without metabolic activation: Sodium azide (TA 1535) 9-Aminoacridine (TA1537, TA 97) 2-(2-Furyl)-3-(5-nitro-2-furyl) acrylamide (TA100, TA98, WP2)
Reference:	MHW, Japan (1997)
Type:	SOS chromotest
System of testing:	<i>Escherichia coli</i> PQ37, PM21, GC4798
Concentration:	Not indicated
Metabolic activation:	With []; Without [X]; With and Without []; No data []
Results:	2,2'-Azobis(2-methylpropanitrile) showed borderline result in PQ37, but negative result in PM21, GC4798.
Cytotoxicity conc:	With metabolic activation: Without metabolic activation:
Precipitation conc:	
Genotoxic effects:	+ ? -
	With metabolic activation: [] [] []
	Without metabolic activation: [] [X] []
Method:	Other
GLP:	Yes [] No [X] ? []
Test substance:	purity: 98 %
Remarks:	
Reference:	Eder <i>et al.</i> : 1989

B. NON-BACTERIAL IN VITRO TEST

Type:	Chromosomal aberration test
System of testing:	Chinese hamster lung (CHL/IU) cells
Concentration:	+S9 mix (short-term treatment): 0, 0.40, 0.80, 1.6 mg/ml -S9 mix (short-term treatment): 0, 0.40, 0.80, 1.6 mg/ml -S9 mix (continuous treatment): 0, 0.40, 0.80, 1.6 mg/ml
Metabolic activation:	With []; Without []; With and Without [X]; No data []
S9:	Rat liver, induced with phenobarbital and 5,6-benzoflavone.
Results:	
Cytotoxicity conc:	Not observed
Precipitation conc:	

Genotoxic effects:	clastogenicity	polyploidy		
	+ ? -	+ ? -		
	With metabolic activation:	[] [] [X]	[] [] [X]	[X]
	Without metabolic activation:	[] [] [X]	[] [] [X]	[X]
Method:	Guide for Screening Mutagenicity Testing of Chemicals (Japan), and OECD TG No. 473			
GLP:	Yes [X] No [] ? []			
Test substance:	purity: 99.9%			
Remarks:	Exposure period: short-term treatment: 6 hr continuous treatment: 24, or 48 hr Positive control: -S9: Mitomycin, +S9: Cyclophosphamide			
Reference:	MHW, Japan (1997)			

* 5.6 GENETIC TOXICITY IN VIVO

No data

5.7 CARCINOGENICITY

No data

*5.8 TOXICITY TO REPRODUCTION

Type:	Fertility []; One-generation study []; Two-generation study []; Other [X]
Species/strain:	Rats/Crj: CD (SD)
Sex:	Female []; Male []; Male/Female [X]; No data []
Route of Administration:	Oral (by gavage)
Exposure period:	Male: From 14 days before mating to 14 days after mating Female: From 14 days before mating to day 3 of lactation
Frequency of treatment:	Daily
Post exposure observation period:	
Premating exposure period:	14 days
Duration of the test:	
Dose:	0, 2, 10, 50 mg/kg/day
Control group:	Yes [X]; No []; No data []; Corn oil Concurrent no treatment[]; Concurrent vehicle[X]; Historical []
NOAEL Parental:	10 mg/kg/day
NOAEL F1 Offspring:	50 mg/kg/day
NOAEL F2 Offspring:	
Results:	

General parental toxicity:

There were no adverse effects of 2,2'-azobis(2-methylpropanitrile) on copulation and fertility, duration of pregnancy, gestation index and parturition at all treated group. Three of 12 dams at 50 mg/kg showed the difficulty of nursing and two of them let all their offsprings die within the first 4 days after birth.

Toxicity to offspring:

This compound showed no adverse effects on viability, sex ratio and body weight gain of pups. However, viability of newborns

at birth and body weight of nurslings on postnatal day 4 was lower than the control levels at 50 mg/kg/day. These changes were considered to be caused by maternal toxicity. There were no morphological abnormalities in pups at all treated groups.

Method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test

GLP: Yes [X] No [] ? []

Test substance: purity: 99.9 %

Remarks:

Reference: MHW, Japan (1997)

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

No data

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

No data

B. Toxicodynamics, toxicokinetics

No data

* 5.11 EXPERIENCE WITH HUMAN EXPOSURE

No data

6. REFERENCES

- *Archiv fuer Toxikologie*. (Berlin, Fed. Rep. Ger.) V.15-31, 1954-74. For publisher formation, see ARTODN. 16, 367 (1957)
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- National Technical Information Service¹. (Springfield, VA 22161) OTS0555369
- National Technical Information Service². (Springfield, VA 22161) AD691-490

Appendix 1.

scenario 1

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m ³]	[kg]	[%]	reaction	advection
air	1,000	7.1.E-06	7.1.E+04	31.0	1.8E+02	7.1.E+02
water	0	4.7.E-03	9.4.E+04	40.9	7.5E+00	9.4.E+01
soil	0	4.0.E-02	6.4.E+04	27.9	5.1E+00	
sediment		4.3.E-03	4.3.E+02	0.2	3.4E-02	8.5.E-03
		total amount	2.3.E+05			

scenario 2

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m ³]	[kg]	[%]	reaction	advection
air	0	4.6.E-07	4.6.E+03	0.5	1.2.E+01	4.6.E+01
water	1000	4.4.E-02	8.7.E+05	98.6	7.0.E+01	8.7.E+02
soil	0	2.6.E-03	4.2.E+03	0.5	3.4.E-01	
sediment		3.9.E-02	3.9.E+03	0.4	3.2.E-01	7.9.E-02
		total amount	8.8.E+05			

scenario 3

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m ³]	[kg]	[%]	reaction	advection
air	0	1.6.E-06	1.6.E+04	0.7	4.1.E+01	1.6.E+02
water	0	3.1.E-02	6.2.E+05	28.6	5.0.E+01	6.2.E+02
soil	1000	9.6.E-01	1.5.E+06	70.6	1.2.E+02	
sediment		2.8.E-02	2.8.E+03	0.1	2.3.E-01	5.7.E-02
		total amount	2.2.E+06			

scenario 4

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m ³]	[kg]	[%]	reaction	advection
air	600	4.6.E-06	4.6.E+04	7.4	1.2.E+02	4.6.E+02
water	300	1.9.E-02	3.8.E+05	61.2	3.1.E+01	3.8.E+02
soil	100	1.2.E-01	1.9.E+05	31.2	1.6.E+01	
sediment		1.7.E-02	1.7.E+03	0.3	1.4.E-01	3.4.E-02
		total amount	6.2.E+05			

Physico-chemical parameter

molecular weight	164.21	Measured	Temp. [°]	25
melting point	101.5	Measured		
vapor pressure [Pa]	8.1E+01	Measured		
water solubility [g/m ³]	350	Measured		
log Kow	1.1	Measured		
half life [h]	in air	272	Estimated	
	in water	8640	Estimated	
	in soil	8640	Estimated	
	in sediment	8640	Estimated	

Environmental parameter

		volume	depth	area	organic	lipid	density	residence
		[m ³]	[m]	[m ²]	carbon [°]	[°]	[kg/m ³]	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

EXTRACT FROM IRPTC LEGAL FILES

File: 17.01 LEGAL**rn : 1645478**

systematic name: Propanenitrile, 2,2'-azobis(2-methyl-
 common name : Azodiisobutyronitrile
 reported name : AZODIISOBUTYRONITRILE
 cas no : 78-67-1
 area : IMO type : REC

subject	specification	descriptor
TRNSP	MARIN	CLASS
LABEL		
PACK		

HAZARD CLASS: 4.1 = INFLAMMABLE SOLID. PACKING GROUP: II = MEDIUM DANGER
 (I=GREAT DANGER - III=MINOR DANGER). SUBSIDIARY RISK LABEL: EXPLOSIVE UN
 NO. 2952

entry date: JAN 1991

amendment: !IMCO*, International Maritime Dangerous Goods Code, , ,
 10004 , 1990

File: 17.01 LEGAL**rn : 1745186**

systematic name: Propanenitrile, 2,2'-azobis(2-methyl-
 common name : Azodiisobutyronitrile
 reported name : AZODIISOBUTYRONITRILE
 cas no : 78-67-1
 area : UN type : REC

subject	specification	descriptor
TRNSP		CLASS
LABEL		
PACK		

HAZARD CLASS: 4.1 = INFLAMMABLE SOLID. PACKING GROUP: II = MEDIUM DANGER
 (I=GREAT DANGER - III=MINOR DANGER). UN NO. 2952

entry date: AUG 1990

amendment: !UNTDG*, UN Transport of Dangerous Goods, Recommendation
 prepared by the Committee of Experts on the Transport of
 Dangerous Goods, , , 15 , 1989