FOREWORD INTRODUCTION

1-CHLOROBUTANE

CAS N°: 109-69-3

SIDS Initial Assessment Report

For

SIAM 6

Paris, France, 9-11 June 1997

1. Chemical Name: 1-Chlorobutane

2. CAS Number: 109-69-3

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

4. Shared Partnership with:

5. Roles/Responsibilities of the Partners:

- Name of industry sponsor /consortium
- Process used

6. Sponsorship History

- How was the chemical or category brought into the OECD HPV Chemicals Programme ?

As a high priority chemical for initial assessment, 1-chlorobutane was selected in the framework of the OECD HPV Chemicals Programme.

SIDS Dossier and Testing Plan were reviewed at a SIDS Review Meeting in 1993, where the following SIDS Testing Plan was agreed:

No testing ( )

Testing (X) Physical-Chemical Properties
- Water solubility
- Partition coefficient

Environmental fate/Biodegradation
- Biodegradation
- Photodegradation
- Stability in water

Ecotoxicity
- Acute toxicity to fish
- Acute toxicity to daphnids
- Toxicity to algae
- Chronic toxicity to daphnids

Toxicity
- Preliminary Reproductive toxicity
- Genotoxicity to bacteria

Chromosomal aberration in vitro

At SIAM-6, the conclusion was approved with comments.
Comments at SIAM-2: Rearrangement of the documents.

7. Review Process Prior to the SIAM:

8. Quality check process:

9. Date of Submission: Date of Circulation: March 1997

10. Date of last Update:

11. Comments:

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	109-69-3
Chemical Name	1-Chlorobutane
Structural Formula	$CH_3CH_2CH_2CH_2$-Cl

CONCLUSIONS AND RECOMMENDATIONS

This chemical does not reveal any remarkable ecotoxicity and PEC/PNEC is lower than 1.

The chemical has some potential for mutagenicity but exposure is assumed to be low.

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

1-Chlorobutane is a stable liquid and its production volume was ca. 800 tonnes/year in 1990 - 1993 in Japan. This chemical is used as an intermediate for the synthesis of catalysts and other organic compounds in closed systems in Japan. The chemical is considered to be "not readily biodegradable". The bioaccumulation factor is 90 - 450.

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 7.3×10^{-9} mg/l (air), 7.4×10^{-7} mg/l (water), 1.2×10^{-5} mg/kg (soil), 7.3×10^{-5} mg/kg (sediment).

For the environment, various NOEC and LC_{50} values were gained from test results; LC_{50} = 120 mg/l (acute fish); EC_{50} = 380 mg/l (acute daphnia); EC_{50} > 1,000 mg/l (acute algae); NOEC = 14 mg/l (long-term daphnia reproduction). Therefore, the chemical is considered to be slightly toxic to fish and daphnids. The lowest chronic toxicity result, 21 d-NOEC (reproduction) of *Daphnia magna* (14 mg/l), was adopted for the calculation of the PNEC, applying an assessment factor of 100. Thus the PNEC of 1-chorobutane is 0.14 mg/l. Since the PEC is lower than the PNEC, environmental risk is presumably low.

The chemical is produced in closed systems, 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 1.5×10^{-4} mg/man/day (i.e. 2.5×10^{-6} mg/kg/day). Also, the daily intake through drinking water is estimated as 2.5×10^{-8} mg/kg/day and through fish is calculated as 7.5×10^{-8} mg/kg/day. No data on occupational exposure are available. Neither monitoring data at work place nor data on consumer exposure have been reported.

The chemical showed no genotoxic effects in bacteria and no chromosomal aberration *in vitro,* while showing positive results in a mouse lymphoma assay.

In a 13-week repeated dose study, mortality and decrease of body weights were observed at the dose of 250 mg/kg/day or more, and these findings might be caused by its irritancy. At the highest dose (500 mg/kg/day), the effects to spleen (e.g. hematopoiesis) were also seen. In a preliminary reproductive/developmental toxicity screening test, the external examination of pups revealed depression of viability index and body weight gain at the highest dose (300 mg/kg/day). All gestation animals which delivered pups had lack of care behaviour in the 12 mg/kg/day group. Salivation was observed in the lowest dose group (2.4 mg/kg/day). Therefore, the NOEL was less than 2.4 mg/kg/day for repeated dose toxicity and 60 mg/kg/day for F1 offspring.

The total exposed dose indirectly through the environment was estimated to be 1.5×10^{-4} mg/man/day (i.e. 2.5×10^{-6} mg/kg/day). Also, the daily intake through drinking water is estimated to be 2.5×10^{-8} mg/kg/day and through fish is calculated to be 7.5×10^{-8} mg/kg/day. For human health, margins of safety by indirect exposure from fish or drinking water are very large. Therefore, health risk is presumably low.

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: 109-69-3		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point			- 123.1 °C
2.2	Boiling Point			78.4 °C (at 1013 hPa)
2.3	Density			3.2 (relative density)
2.4	Vapour Pressure		OECD TG 104	136.5 hPa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	2.82 at 25 °C
2.6 A.	Water Solubility		OECD TG 105	370 mg/L 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		estimation	$T_{1/2}$ = 9.6 y (direct photolysis in water)
3.1.2	Stability in Water		OECD TG 111	Not measurable
3.2	Monitoring Data			No data available
3.3	Transport and Distribution		Calculated (MNSEM-147S)	In Air 7.3E-9 mg/L In Water 7.4E-7 mg/L In Soil 1.2E-5 mg/kg In Sediment 7.3E-5 mg/kg
3.5	Biodegradation		OECD TG 301C	Not readily biodegradable: 0 % (BOD) in 28 days.
3.6	Bioaccumulation	Carp	OECD TG 305C	BCF: 90 – 450
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oryzias latipes*	OECD TG 203	LC_{50} (96hr): 120 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50} (24hr): 380 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD TG 201	EC_{50} (72hr): > 1,000 mg/l
4.5.2	Chronic Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50} (21d, Mortality): 60 mg/l EC_{50} (21d, Reproduction): 40 mg/l NOEC(21d, Repro): 14 mg/l
4.6.1	Toxicity to Soil Dwelling Organisms			No data available.
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		LD_{50}: 2,670 mg/kg
5.1.2	Acute Inhalation Toxicity	Rat		LCLo: 8,000 ppm
5.1.3	Acute Dermal Toxicity			LD_{50}: >20 ml/kg
5.4	Repeated Dose Toxicity	Rat	NTP (13 weeks)	NOAEL = 120 mg/kg/day
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	*S. .typhimurium* *E. coli*	OECD T G471 and 472 andJapanese Guidelines	Negative (With metabolic activation) Negative (Without metabolic activation)

CAS NO: 109-69-3		SPECIES	PROTOCOL	RESULTS
B.	Non-Bacterial In Vitro Test (Chromosomal aberrations)	CHL cells	OECD TG 473 and Japanese Guidelines	negative(With metabolic activation) negative(Without metabolic activation)
5.6	Genetic Toxicity In Vivo			No data available.
5.8	Toxicity to Reproduction	Rat	OECD Combined Test	NOEL Parental = < 2.4 mg/kg/day NOEL F1 offspring = 60 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity			
5.11	Experience with Human Exposure			

SIDS Initial Assessment Report

1 IDENTITY

1.1 Identification of the Substance

CAS Number: 109-69-3
IUPAC Name: 1-Chlorobutane
Molecular Formula: C_4H_9Cl
Structural Formula: $CH_3CH_2CH_2CH_2Cl$

Synonyms: Butyl chloride

1.2 Purity/Impurities/Additives

Degree of Purity: 99.9 %

Major Impurities: Isobutyl chloride

2-Chlorobutane

Butanol

Essential Additives: No additives

1.3 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

Property	Value
Melting point	-123.1 °C
Boiling point	78.4 °C
Vapour pressure	136.5 hPa at 25 °C
Water solubility	370 mg/l at 25 °C
Partition coefficient n-octanol/water (log value)	2.82

2 GENERAL INFORMATION ON EXPOSURE

2.1 Production Volumes and Use Pattern

1-Chlorobutane is a stable liquid, and the production volume was ca. 800 tonnes/year in 1990 - 1993 in Japan. This chemical is used as an intermediate for the synthesis of catalysts and other organic compounds in closed systems in Japan. Release to the environment may occur at the production site, as well as specific industrial sites. All of disposal wastes are treated by incineration. 1-Chlorobutane seems to be released into water and air from its production sites after biological treatment. No specific monitoring data of the chemical are available. This chemical is classified as "not readily biodegradable".

2.2 Environmental Exposure and Fate

2.2.1 Photodegradation

The half-life time of 9.6 years is estimated for the degradation of 1-chlorobutane in water by direct photolysis. (MITI, Japan).

2.2.2 Stability in Water

No data are available.

2.2.3 Biodegradation

If released into water, this substance is not readily biodegraded (MITI (I), corresponding to the OECD 301C: 0 % degradation during 28 days based on BOD).

2.2.4 Bioaccumulation

BCF= 90 – 450 in carp (6 weeks at 25 °C) suggests that the potential for bioconcentration in aquatic organisms is low (MITI, Japan, 1992).

2.2.5 Estimates of environmental fate, pathway and concentration

The potential environmental distribution of 1-chlorobutane obtained from a generic fugacity model, Mackay level III, under emission scenarios is shown below. The results show that when 1-chlorobutane is released into water, the majority of the chemical is likely distributed into soil and sediment

PECs have been calculated based on several models (MNSEM, CHEMCAN, CHEMFRN) considering its physico-chemical properties (e.g. molecular weight, water solubility, vapour pressure and partition coefficient). The estimated concentrations with the MNSEM model were 7.3×10^{-9} mg/l (air), 7.4×10^{-7} mg/l (water), 1.2×10^{-5} mg/kg (soil), 7.3×10^{-5} 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 1.5×10^{-4} mg/man/day (i.e. 2.5×10^{-6} mg/kg/day). Also, the daily intake through drinking water is estimated as 2.5×10^{-8} mg/kg/day and through fish is calculated as 7.5×10^{-8} mg/kg/day.

Global situation:

Method: MNSEM 147S

Input data:	Molecular weight:	92.57
	Water solubility:	370.00 [mg/l]
	Vapor pressure:	7.9E+01 [mmHg]
	Log Pow:	2.82

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

Air:	7.3E-09 [mg/l]	
Water:	7.4E-07 [mg/l]	
Soil:	1.2E-05 [mg/kg dry solid]	
Sediment:	7.3E-05 [mg/kg dry solid]	

Exposure dose

Inhalation of air:	1.5E-04 [mg/day]	
Drinking water:	1.5E-06 [mg/day]	(2.5E-08 mg/kg/day)
Ingestion of fish:	4.5E-06 [mg/day]	(7.5E-08 mg/kg/day)
meat:	9.7E-11 [mg/day]	
milk:	1.2E-10 [mg/day]	
vegetation:	8.1E-07 [mg/day]	
Total exposure dose:	1.5E-04 [mg/day]	(2.5 E-6 mg/kg/day)

Remarks: 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

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	7.3E-09	7.4E-07	1.2E-05	7.3E-05
CHEMCAN2	1.2E-07	6.0E-07	1.6E-06	9.7E-06
CHEMFRAN	1.2E-07	6.1E-07	1.6E-06	1.0E-05

2.3 Human Exposure

2.3.1 Occupational Exposure

No data on work place monitoring have been reported.

2.3.2 Consumer Exposure

No data on consumer exposure are available.

3 HUMAN HEALTH HAZARDS

3.1 Effects on Human Health

3.1.1 Acute Toxicity

Oral and dermal LD_{50} values of 1-chlorobutanefor male rats were reported as 2,670 mg/kg and > 20 ml/kg, respectively. Inhalation LCLo was reported as 8,000 ppm. Two reports on irritation tests are available. According to these results, 1-chlorobutane was moderately to highly irritating to skin and slightly irritating to eyes in rabbits.

3.1.2 Repeated Dose Toxicity

There is an NTP study on 14 days and 13 week repeated dose toxicity study in rats of 1-chlorobutane (US/NTP, 1986). As the study was well controlled and conducted under GLP, this was appropriate to regard as a key study.

Male and female F344/N rats were orally administered (gavage) at doses of 0, 190, 380, 750, 1,500 and 3,000 mg/kg/day for 14 days. All the rats that received 1500 or 3000 mg/kg and 3/5 males and 1/5 females that received 750 mg/kg died before the end of the studies. No gavage accidents were noted, therefore, all deaths were considered compound related. The final mean body weight of the male and female rats that received 750 mg/kg was 14% and 6% lower than that of vehicle controls, respectively. Convulsions were observed in males that received 750 mg/kg or more groups and in one female that received 1500 mg/kg. Aggressiveness and hyperactivity were observed in rats that received 750 mg/kg. A bloody discharge from the nose and mouth was observed in males that received 750 mg/kg or more and females that received 1500 mg/kg. At necropsy, blood was found in the cranial cavity of males that received 750 mg/kg or more and females that received 1500 mg/kg or more. Histologic examinations were not performed.

The NOAEL for 14 days repeated dose toxicity in rats is considered to be 380 mg/kg/day.

Male and female F344/N rats were orally administered (gavage) at doses of 0, 30, 60, 120, 250 and 500 mg/kg/day for 13 weeks. Six of 10 male rats that received 500 mg/kg died before the end of studies. Because of the increased irritability of rats at the higher doses, dosing by gavage became extremely difficult; three deaths occurred in the 500 mg/kg group because of gavage accidents. The final mean body weights of males that received 250 and 500 mg/kg were 11% or 20% lower than that of the vehicle controls. Final mean body weights of females that received 250 and 500 mg/kg were 6% or 10% lower than controls. Five of 10 males and 2/10 females that received 250 or 500 mg/kg males and 8/10 females that received 500 mg/kg had convulsions on one or more occasions. Extramedullary hematopoiesis of the spleen was observed in 3/10 males that received 500 mg/kg. The severity was mild in two rats and moderate in a third. This lesion was not observed in vehicle control animals.

The NOAEL for repeated dose toxicity in rats is considered to be 120 mg/kg/day.

3.1.3 Mutagenicity

In vitro Studies

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 the pre-incubation

method. This study was well controlled and regarded as a key study. 1-Chlorobutane showed negative results in *Salmonella typhimurium* TA100, TA1535, TA98, TA1537 and *Escherichia coli* WP2 *uvr*A at concentrations up to 78 ug/plate with or without a metabolic activation system (MHW, 1993).

Also, an NTP study showed negative results in *Salmonella typhimurium* TA100, TA1535, TA98, TA1537, TA1538 with or without a metabolic activation system (NTP, 1986).

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 within no apparent cytotoxic effect in continuous treatment. In short term treatment, it was set to 3.5 mg/ml because the concentration was equivalent to ca. 10 mM as required in test guidelines. No structural chromosomal aberrations or polyproidy were recognized up to a maximum concentration of 0.93 mg/ml under conditions of both continuous treatment and short-term treatment with or without an exogeneous metabolic activation system (MHW, 1993). Also, an NTP study using Chinese Hamster ovary (CHO) cells showed negative results with or without an exogeneous metabolic activation system (NTP, 1986) up to 5.0 mg/ml concentration.

On the other hand a mouse lymphoma assay proved to be positive without metabolic activation (NTP, 1986)

In vivo Studies

No data are available on *in vivo* genotoxic effects.

3.1.4 Carcinogenicity

In an NTP carcinogenicity assay in rats and mice, 1-chlorobutane showed no evidence of carcinogenicity for male and female rats at doses of 60 or 120 mg/kg/day, or mice at doses of 250, 500, 1,000 mg/kg/day (NTP, 1986).

3.1.5 Toxicity for Reproduction

1-Chlorobutane was studied for oral toxicity in rats according to the OECD preliminary reproduction toxicity test at doses of 0, 2.4, 12, 60 and 300 mg/kg/day. Although this study was designed to investigate reproductive capability in parental generation as well as development in F_1 offspring, parameters to evaluate reproductive toxicity were limited to only body weights at day 0 and day 4 after birth, and autopsy findings at day 4.

Regarding the effects to parents, depression of body weight gain and 2 females death were observed in 300 mg/kg group. In the clinical observations, salivation was observed in all chemical treatment groups. No change was observed in gross and histopathological findings, and organ weights in males of each treatment group.

Erosion and desquamation were seen on mucous in glandular stomach of 300 mg/kg females. The results observed in mating, fertility and estrous cycle did not reveal any effects attributable to the administration of the chemical. Observation of delivery revealed that all gestation animals delivered pups normally and there were lack of care in behavior in the 12 mg/kg groups or more. The external examination of pups revealed depression of viability index and body weight gain in the 300 mg/kg

group. Thus the NOEL was considered to be < 2.4 mg/kg/day for reproduction in parent animals and 60 mg/kg/day for the F1 generation.

3.2 Initial Assessment for Human Health

The chemical is produced 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 1.5×10^{-4} mg/man/day (i.e. 2.5×10^{-6} mg/kg/day). Also, the daily intake through drinking water is estimated as 2.5×10^{-8} mg/kg/day and through fish is calculated as 7.5×10^{-8} mg/kg/day. No data on occupational exposure are available. Neither monitoring data at work place nor data on consumer exposure have been reported.

The chemical showed no genotoxic effects in bacteria and no chromosomal aberration *in vitro,* while showing positive results in a mouse lymphoma assay. In an NTP carcinogenicity assay in rats and mice, 1-chlorobutane showed no evidence of carcinogenicity for male and female rats at doses of 60 or 120 mg/kg/day, or mice at doses of 250, 500, 1,000 mg/kg/day.

In a 13-week repeated dose study, mortality and decrease of body weights were observed at the dose of 250 mg/kg/day or more, and these findings might be caused by its irritancy. At the highest dose (500 mg/kg/day), the effects to spleen (e.g. ematopoiesis) were also seen. The NOAEL of this study is considered to be 120 mg/kg/day.

In a preliminary reproductive/ developmental toxicity screening test, the external examination of pups revealed depression of viability index and body weight gain at the highest dose (300 mg/kg/day). All gestation animals which delivered pups had lack of care behaviour in the 12 mg/kg/day group. Salivation was observed in the lowest dose group (2.4 mg/kg/day). Therefore, the NOEL was less than 2.4 mg/kg/day for repeated dose toxicity and 60 mg/kg/day for F1 offspring.

The total exposed dose indirectly through the environment was estimated as 1.5×10^{-4} mg/man/day (i.e. 2.5×10^{-6} mg/kg/day). Also, the daily intake through drinking water is estimated as 2.5×10^{-8} mg/kg/day and through fish is calculated as 7.5×10^{-8} mg/kg/day. For human health, margin of safety by indirect exposure from fish or drinking water are very large. Therefore, the health risk is presumably low.

4 HAZARDS TO THE ENVIRONMENT

4.1 Aquatic Effects

Ecotoxicity

1-Chlorobutane 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,]. Acute and chronic toxicity data to test organisms for 1-chlorobutane are summarized in Table 2. No other ecotoxicological data are available.

Various NOEC and LC_{50} values were gained from these tests; 96h LC_{50} = 120 mg/l (acute fish); 24h EC_{50} = 380 mg/l (acute daphnia); 72h EC_{50} = >1,000 mg/l (acute algae); 21d NOEC = 14 mg/l (long-term daphnia reproduction). Therefore, the chemical is considered to be slightly toxic to fish, daphnids and non-toxic to algae.

A toxicity to bacteria was available; EC10 = 332.3 mg/l [DIN 38412 part8, *Pseudomonas putida*, 18hr](Huels AG, unpublished data).

As the lowest chronic toxicity result, the 21 d-NOEC (reproduction) of *Daphnia magna* (14 mg/l) was adopted. An assessment factor of 100 is applied. Thus the PNEC of 1-chlorobutane is 0.14 mg/l. Since the PEC is lower than the PNEC, the environmental risk is presumably low.

Table 2 Acute and chronic toxicity data of 1-chlorobutane to aquatic organisms.

Species	Endpoint*1	Conc. (mg/L)	Reference
Selenastrum capricornutum (algae)	Biomass: EC_{50} (72h)	> 1,000 mg/L	EA , Japan. (1992)
Daphnia magna (water flea)	Imm: EC_{50}(24h) Mor: LC_{50}(21d) Rep: EC_{50}(21d) NOEC(21d)	380 mg/L 60 mg/L 40 mg/L 14 mg/L	EA , Japan. (1992)
Oryzias latipes (fish, Medaka) Poecilia reticulate (guppy)	Mor: LC_{50}(96h) Mor: LC50(7d)	120 mg/L 96.9 mg/L	EA , Japan. (1992) Koenemann (1981)
Species	Endpoint *1	Conc. (mg/L)	Reference
Selenastrum capricornutum (algae)	Biomass: EC50 (72h)	> 1,000 mg/L	EA , Japan. (1992)
Daphnia magna (water flea)	Imm: EC50(24h) Mor: LC50(21d) Rep: EC50(21d) NOEC(21d)	380 mg/L 60 mg/L 40 mg/L 14 mg/L	EA , Japan. (1992)
Oryzias latipes (fish, Medaka) Poecilia reticulate (guppy)	Mor: LC50(96h) Mor: LC50(7d)	120 mg/L 96.9 mg/L	EA , Japan. (1992) Koenemann (1981)

Notes: *1 Mor; mortality, Rep; reproduction. Imm; immobilisation

4.2 Initial Assessment for the Environment

1-Chlorobutane is a stable liquid and the production volume was ca. 800 tonnes/year in 1990 - 1993 in Japan. This chemical is used as an intermediate for the synthesis of catalysts and other organic compounds in closed systems in Japan. The chemical is considered as "not readily biodegradable". The bioaccumulation factor is 90 – 450 in carp.

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 7.3×10^{-9} mg/l (air), 7.4×10^{-7} mg/l (water), 1.2×10^{-5} mg/kg (soil), 7.3×10^{-5} mg/kg (sediment).

For the environment, various NOEC and LC_{50} values were gained from test results; 96h LC_{50} = 120 mg/l (acute fish); 24h EC_{50} = 380 mg/l (acute daphnia); 72h EC_{50} > 1,000 mg/l (acute algae); 21d NOEC = 14 mg/l (long-term daphnia reproduction). Therefore, the chemical is considered to be slightly toxic to fish and daphnids. The lowest chronic toxicity result, 21 d-NOEC (reproduction) of *Daphnia magna* (14 mg/l), was adopted for the calculation of the PNEC, applying an assessment factor of 100. Thus the PNEC of 1-chorobutane is 0.14 mg/l. Since the PEC is lower than the PNEC, the environmental risk is presumably low.

5 RECOMMENDATIONS

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

This chemical does not reveal any remarkable ecotoxicity and PEC/PNEC is lower than 1.

The chemical has some potential for mutagenicity but exposure is assumed to be low.

6 REFERENCES

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SIDS DOSSIER

1-Chlorobutane

CAS No. 109-69-3

Sponsor Country: Japan

S I D S P R O F I L E

1.01 A.	**CAS No.**	109-69-3
1.01 C.	**CHEMICAL NAME (OECD Name)**	1-Chlorobutane
1.01 D.	**CAS DESCRIPTOR**	Not applicable
1.01 G.	**STRUCTURAL FORMULA**	C_4H_9Cl
	OTHER CHEMICAL IDENTITY INFORMATION	$CH_3CH_2CH_2CH_2Cl$
1.5	**QUANTITY**	In Japan approx. 800 tonnes in 1990 - 1993.
1.7	**USE PATTERN**	(a) Intermediate for catalyst in Japan (97 - 100%) (b) Specialty solvent or intermediate for organic synthesis
1.9	**SOURCES AND LEVELS OF EXPOSURE**	1. Amount released from production site to water is < 8 kg/year in Japan. Diluted wastes water (< 2mg/l) is released. 2. Amount released to air from production site is < 1,500 kg/year All of the waste gas is treated by absorption tower and scrubber, and then released
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)		

S I D S S U M M A R Y

CAS NO: 109-69-3		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	Y	N	N	Y	N	Y	N
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	Y	Y	Y	N	N	Y	N
5.5	Genetic Toxicity *in vitro*							
	. Gene mutation	Y	Y	Y	N	N	Y	N
	. Chromosomal aberration	Y	Y	Y	N	N	Y	N
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								

1.01 SUBSTANCE INFORMATION

A.	**CAS-Number**	109-69-3
B.	**Name** *(IUPAC name)*	Butyl chloride
C.	**Name** *(OECD name)*	1-Chlorobutane
D.	**CAS Descriptor**	Not applicable
E.	**EINECS-Number**	203-696-6
F.	**Molecular Formula**	C_4H_9Cl
G.	**Structural Formula**	
		$CH_3CH_2CH_2CH_2Cl$
H.	**Substance Group**	Not applicable
I.	**Substance Remark**	
J.	**Molecular Weight**	92.57

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 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

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

C. Purity 99.9 % (weight/weight)

1.2 SYNONYMS Butyl chloride

1.3 IMPURITIES (a) Name: iso-Butyl chloride
(b) Name: 2-Chlorobutane
(c) Name: n-Butanol

1.4 ADDITIVES None

1.5 QUANTITY

Location	Production (tonnes)	Date
Japan	800	1990-1993

Export (tonnes)	1993	1992	1991	1990
U.S.A.	500	370	210	230
China	40	80	40	0
Indonesia	40	20	0	0
England	100	0	100	100

Reference: MITI, Japan

1.6 LABELLING AND CLASSIFICATION

Labelling None

Classification None

1.7 USE PATTERN

A. General

	Type of Use:	**Category:**
	(a) main industry use	Intermediate for catalyst (Closed system) 97 - 100 %
	(b) main industry use	Direct use: Specialty solvent Indirect use: Intermediate for organic synthesis

Remarks: None

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

B. Uses in Consumer Products

None

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Source:	Number of workers	Frequency & duration	Emission
Maintenance	1	30 min/2 day	< 10 mg/m^3

Reference: MITI, Japan

1.9 SOURCES OF EXPOSURE

(a)
Source: Media of release: Water from a production site
Quantities per media: < 8 kg/year
Remarks: Diluted wastes water (< 2 mg/l) is released.

(b)
Source: Media of release: Air from a production site
Quantities per media: < 1,500 kg/year
Remarks: All of the waste gas are treated by absorption tower and scrubber, and then released.

Reference: MITI, Japan

1.10 ADDITIONAL REMARKS

A. Options for disposal None

B. Other remarks None

2.1 MELTING POINT

Value:	- 123.1 °C
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Remarks:	None
Reference:	Weissberger, A.

2.2 BOILING POINT

Value:	78.44 °C
Pressure:	at 1013.3 hPa
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:	
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	None
Reference:	Weissberger, A.

2.3 DENSITY (Relative density)

Type:	Bulk density **[ ]**; Density **[ ]**; Relative Density **[X]**
Value:	3.2
Temperature:	
Method:	Unknown
GLP:	Yes [ ] No **[ ]** ? **[X]**
Remarks:	
Reference:	ECDIN Database

2.4 VAPOUR PRESSURE

Value:	102.4 Torr (136.5 hPa)
Temperature:	25 °C
Method:	calculated **[ ]**; measured [X]
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	None
Reference:	Driesbach, R.R, (1961)

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

Log Pow:	2.82
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:	370 mg/l
Temperature:	25 °C
Description:	Miscible**[ ]**; Of very high solubility **[ ]**;

	Of high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[X]**; Of very low solubility **[ ]**; Not soluble **[ ]**
Method:	OECD Test Guideline 105 Flask
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Remarks:	None
Reference:	MITI, Japan (1993)

B. pH Value, pKa Value

No studies located

2.7 FLASH POINT

Value:	- 6.7 °C
Type of test:	Closed cup **[ ]**; Open cup **[ ]**; Other **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	None
Reference:	Source Book of Industrial Solvents (1957)

2.8 AUTO FLAMMABILITY

Not applicable

2.9 FLAMMABILITY

Value:	Flame point: 460 °C
Results:	Extremely flammable **[ ]**;Extremely flammable-liquified gas **[]**; Highly Flammable **[ ]**; Flammable **[ ]**; Non flammable **[ ]**; Spontaneously flammable in air **[ ]**; Contact with water liberates highly flammable gases **[ ]**; Other **[ ]**
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	Flammable limits: LEL 1.9 % UEL 10.1 %
Reference:	Weissberger, A.

2.10 EXPLOSIVE PROPERTIES

No studies located

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

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 = 3.52 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	$.14 \times 10^{-13}$ mol/l/s
	Half life	9.60 years
Reference	Lyman, W. J., et al. (1981)	

3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[ ]**; biotic (sediment)**[ ]**
Half life:
Method:
GLP: Yes **[ ]** No **[ ]** ? **[ ]**
Test substance:
Remarks: Unmeasureable (evaporated)
Reference:

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:	7.3E-09 [mg/l]
Water:	7.4E-07 [mg/l]
Soil:	1.2E-05 [mg/kg dry solid]
Sediment:	7.3E-05 [mg/kg dry solid]

Exposure dose

Inhalation of air:	1.5E-04 [mg/day]
Drinking water:	1.5E-06 [mg/day]
Ingestion of fish:	4.5E-06 [mg/day]
meat:	9.7E-11 [mg/day]
milk:	1.2E-10 [mg/day]
vegetation:	8.1E-07 [mg/day]

Total exposure dose: 1.5E-04 [mg/day]

Remarks: Input data:

Molecular weight:	92.57
Water solubility:	370.00 [mg/l]
Vapor pressure:	7.9E+01 [mmHg]
Log Pow:	2.82

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

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	7.3E-09	7.4E-07	1.2E-05	7.3E-05
CHEMCAN2	1.2E-07	6.0E-07	1.6E-06	9.7E-06
CHEMFRAN	1.2E-07	6.1E-07	1.6E-06	1.0E-05

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]**;
Concentration of the chemical:	5.18 mg/l related to COD **[ ]**; DOC **[ ]**; Test substance **[X]**
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[X]**; others **[ ]**
Degradation:	0 % after 28 days
Results:	Readily biodeg. **[ ];** Inherently biodeg. **[ ]**; under test condition no biodegradation observed **[X]**, Other **[ ]**
Method:	OECD Test Guideline 301D
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	1-Chlorobutane

Remarks: None
Reference: MITI, Japan (1992)

3.6 BOD_5,COD OR RATIO BOD_5/COD

No studies located

3.7 BIOACCUMULATION

Species:	Carp
Exposure period:	6 weeks
Temperature:	25 °C
Concentration:	(1) 0.36 mg/l (2) 0.036 mg/l
BCF:	(1) 90 - 110 (2) 300 - 450
Elimination:	Yes **[ ]** No **[ ]** ? **[ ]**
Method:	OECD Test Guideline 305C
Type of test:	calculated; **[X]** measured **[ ]** static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	1-Chlorobutane, Purity: > 99 %
Remarks:	None
Reference:	MITI, Japan (1992)

3.8 ADDITIONAL REMARKS None

A. Sewage treatment

B. Other information

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) = 120 mg/l (95% confidence level: 110-130 mg/l) LC_{50} (48h) = 120 mg/l (95% confidence level: 110-130 mg/l) LC_{50} (72h) = 120 mg/l (95% confidence level: 110-130 mg/l) LC_{50} (96h) = 120 mg/l (95% confidence level: 110-130 mg/l) NOEC = LOEC =
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	OECD Test Guideline 203 (1981)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	1-Chlorobutane, Purity = 98.8 %
Remarks:	A group of 10 O*ryzias latipes* were exposed to 5 nominal Concentrations (63-180 mg/l)
Reference:	EA, Japan (1993)

(b)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[ ]**; closed-system **[ ]**
Species:	*Poecilia reticulata* (Guppy)
Exposure period:	7 days
Results:	LC_{50} (7d) = 96.9 mg/l NOEC = LOEC =
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	Unknown
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	1-Chlorobutane
Remarks:	
Reference:	Koenemann, H. (1981)

(c)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[ ];** other **[ ];** open-system **[ ]** closed-system **[ ]**
Species:	*Leuciscus idus* (Goldorfe)
Exposure period:	48 hrs
Results:	LC_{50} (48h) = 245 mg/l LC_{0} (48h) = 200 mg/l NOEC = LOEC =
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	DIN 38412 Part 15
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	1-Chlorobutane
Remarks:	
Reference:	Unpublished Report (Germany)

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) = 380 mg/l (95% confidence level: 310-480 mg/l) EC_{50} (48h) = NOEC = LOEC =
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	OECD Test Guideline 202 (1984)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	1-Chlorobutane, purity: = 98.8 %
Remarks:	20 daphnids (4 replicates; 5 organisms per replicate) were exposed to 5 nominal concentrations (100-1000 mg/l)
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) = > 1000 mg/l NOEC = LOEC =
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**	
Method:	open-system **[**X**]**; closed-system **[ ]** OECD Test Guideline 201 (1984)	
GLP:	Yes **[ ]** No **[X]** ? **[ ]**	
Test substance:	1-Chlorobutane, purity = 98.8 %	
Remarks:	The EC_{50} values were calculated based on 5 nominal Concentrations (95-1000 mg/l)	
Reference:	EA, Japan (1992)	

4.4 TOXICITY TO BACTERIA

Type:	Aquatic **[ ]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:	*Pseudomonas putida*
Exposure Period:	18 hrs
Results:	EC_{10} (18 hour) = 332.3 mg/l
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	DIN 38412 Part 8
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	1-Chlorobutane
Remarks:	
Reference:	Unpublished report (Huels AG)

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1. CHRONIC TOXICITY TO FISH

No studies located

4.5.2. CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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) = 330 mg/l (95% confidence level:280-410 mg/l)
	LC_{50} (48 h) = 190 mg/l (95% confidence level:160-220 mg/l)
	LC_{50} (96 h) = 110 mg/l (95% confidence level: 95-130 mg/l)
	LC_{50} (7 d) = 110 mg/l (95% confidence level: 88-120 mg/l)
	LC_{50} (14 d) = 77 mg/l (95% confidence level: 59-100 mg/l)
	LC_{50} (21 d) = 60 mg/l (95% confidence level: 50- 77 mg/l)
	NOEC =
	LOEC =
Reproduction:	EC_{50} (14 d) = 29 mg/l (95% confidence level: 19-44 mg/l)
	EC_{50} (21 d) = 40 mg/l (95% confidence level: 31-52 mg/l)
	NOEC = 14 mg/l ($P < 0.05$)
	LOEC = 46 mg/l ($P < 0.05$)
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	OECD Test Guideline 202 (1984)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	1-Chlorobutane, purity = 98.8 %
Remarks:	40 daphnids (4 replicates; 10 organisms per replicate) were exposed to 5 nominal concentrations (4.6-460 mg/l)
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

5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type :	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Rat
Value :	2,670 (mg/kg):
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	1-Chlorobutane, purity: unknown
Remarks:	None
Reference:	Smyth H. et al. (1954)

5.1.2 ACUTE INHALATION TOXICITY

Type :	LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[X]**; Other **[ ]**
Species/strain:	Rat
Exposure time:	
Value:	8,000 ppm
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	1-Chlorobutane
Remarks:	
Reference:	Smyth, H. et al. (1954)

5.1.3 ACUTE DERMAL TOXICITY

Type :	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[ ]**; LDL_0 **[X]**; Other **[ ]**
Species/strain:	
Value:	> 20 ml/kg
Method:	Unknown
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	
Comments:	
Remarks:	
Reference:	Smyth, H. et al. (1954)

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

No studies located

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

Species/strain: Rabbit

Results:	(1) 10mg 24H open Mild (2) 500mg 24h open mild Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[X]**; Irritating **[ ]**; Moderate irritating **[X]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Highly corrosive (causes severe burns) **[ ]**; Corrosive (caused burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**
Method:	1) Open Draize Test 2) Standard Draize Test

GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: 1-Chlorobutane, purity: unknown
Remarks:
Reference: 1) Arch. Ind. Hygiene Occup. Med. (1954)
2) Marhold, J.P.P. (1986)

5.2.2 EYE IRRITATION/CORROSION

Species/strain: Rabbit
Results: (1) 500 mg
(2) 500 mg 24H Mild
Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[X]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: Irritating **[ ]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: 1) Open Draize Test
2) Standard Draize Test
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance:
Remarks: None
Reference: 1) Arch. Ind. Hygiene Occup. Med. (1954)
2) Marhold, J.P.P. (1986)

5.3 SKIN SENSITISATION

No studies located

5.4 REPEATED DOSE TOXICITY

(a)
Species/strain: Rat (F344/N)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: oral (gavage)
Exposure period: 14 days
Frequency of treatment: 7 days/week
Post exposure observation period:
Dose: 0, 190, 380, 750, 1500 or 3000 mg/kg (5 animals /group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL: 380 mg/kg
LOEL: 750 mg/kg
Results: All the rats that received 1500 or 3000 mg/kg and 3/5 males and 1/5 females that received 750 mg/kg died before the end of the studies. No gavage accidents were noted, therefore, all deaths were considered compound related. The final mean body weight of the male and female rats that received 750 mg/kg was 14% and 6% lower than that of vehicle controls, respectively. Convulsions were observed in males that received 750 mg/kg or more groups and in one female that received 1500 mg/kg. Aggressiveness and hyperactivity were observed in rats that received 750 mg/kg. A bloody discharge from the nose and mouth was observed in males that received 750 mg/kg or more and females that received 1500 mg/kg. At necropsy, blood was found in the cranial cavity of males that received 750 mg/kg or more and females that received 1500 mg/kg or more. Histologic examinations were not performed.
Method: NTP study

GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Purity: > 99.5 %
Reference: US/NTP (1986)

(b)
Species/strain: Rat (F344/N)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: oral (gavage)
Exposure period: 13 weeks
Frequency of treatment: 5 days/week
Post exposure observation period:
Dose: 0, 30, 60, 120, 250 or 500 mg/kg (10 animals /group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL: 120 mg/kg
LOEL: 250 mg/kg
Results: Six of 10 male rats that received 500 mg/kg died before the end of studies. Because of the increased irritability of rats at the higher doses, dosing by gavage became extremely difficult; three death occurred in the 500 mg/kg group because of gavage accidents. The final mean body weights of males that received 250 and 500 mg/kg were 11% or 20% lower than that of the vehicle controls. Final mean body weights of females that received 250 and 500 mg/kg were 6% or 10% lower than controls. Five of 10 males and 2/10 females that received 250 or 500 mg/kg males and 8/10 females that received 500 mg/kg had convulsions on one or more occasions. Extramedullary hematopoiesis of the spleen was observed in 3/10 males that received 500 mg/kg. The severity was mild in two rats and moderate in a third. This lesion was not observed in vehicle control animals.
Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Commercial, purity: > 99.5 %
Reference: US/NTP (1986)

(c)
Species/strain: Rat (F344/N)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral (gavage)
Exposure period: 103 weeks
Frequency of treatment: 5 days/week
Postexposure observation period:
Doses: 0, 60, 120 (50 animals/group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL: 60 mg/kg
LOEL: 120 mg/kg
Results: Survival relative to that of vehicle controls was significantly lower in high dose male rat (40/50) vs 17/50) and high dose female rats (35/50 vs 11/50). No adverse effects on survival or body weights in other dosed groups of rats were observed. Convulsions were observed before or after gavage administration on several occasions during the study.
These observations were noted primarily in the high dose group. Hemorrhage of the brain and alveoli were observed primarily in high dose male and female rats dying from convulsions. Lymphoid depletion

of the spleen and splenic hemosiderosis were also observed in these animals.

Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance:Purity: > 99.5 %
Remarks:
Reference: US/NTP (1986)

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
E. coli uvrA
Concentration: 0, 2.4 - 78.12 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: 78.12 µg/plate
Without metabolic activation: 78.12 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: 99.7 %
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 (1993b)

(b)
Type : Bacterial reverse mutation assay
System of testing: Species/strain: *S. typhimurium* TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration: 0, 10 - 666 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Genotoxic effects:

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

Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Teat substance:Purity: > 99.5 %
Remarks: Procedure: Pre-incubation.
Reference: US/NTP (1986)

B. NON-BACTERIAL IN VITRO TEST

(a)
Type : Cytogenetics Assay
System of testing: Species/strain: Chinese hamster CHL cells
Concentration: Incubated with 0, 0.23 - 0.93 mg/ml (+S9)
0, 0.23 - 0.93 mg/ml (-S9)
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: > 0.93 mg/ml
Without metabolic activation: > 0.93 mg/ml
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 **[ ]** ? **[ ]**
Test substance: Commercial, purity > 99.5 %
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
No. replicates: 1
Reference: MHW, Japan (1993b)

(b)
Type : Cytogenetics Assay
System of testing: Species/strain: Chinese hamster CHO cells
Concentration: Incubated with 0, 1600 -5000 µg/ml
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Genotoxic effects:

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

Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Purity > 99.5 %
Remarks: Plates/test: 2
Activation system: S-9 fraction from the liver of Arochlor 1254 induced male SD derived rats with NADPH-generating system
No. replicates: 1
Reference: US/NTP (1986)

(c)
Type : Sister chromatid exchanges
System of testing: Species/strain: Chinese hamster CHO cells
Concentration: Incubated with 0, 500 - 5000 µg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Genotoxic effects:

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

Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance:Purity > 99.5 %
Remarks: Plates/test: 2
Activation system: S-9 fraction from the liver of Arochlor 1254 induced male SD derived rats with NADPH-generating system
No. replicates: 1
Reference: US/NTP (1986)

(d)
Type : Mouse lymphoma assay
System of testing: Species/strain: L5178Y/YK+/- Mouse Lymphoma cells
Concentration: Incubated with 0, 350 - 550 µg/plate
Metabolic activation: With **[ ]**; Without **[X]**; With and Without **[ ]**; No data **[ ]**
Results:

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

Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance:Purity > 99.5 %
Remarks:
Reference: US/NTP (1986)

5.6 GENETIC TOXICITY IN VIVO

No studies located

5.7 CARCINOGENICITY

Species/strain: Rat (F344/N) and mice ($B6C3F_1$)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral (gavage)
Exposure period: 103 weeks
Frequency of treatment: 5 days/week
Post-exposure observation period:
Doses: 0, 250, 500, 1,000 mg/kg/day
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**;
Historical **[ ]**
Results: There is no evidence of carcinogenicity of butyl chloride for male and female F344/N rats at daily doses of 60 or 120 mg/kg, for male B6C3F1 mice at doses of 250, 500 or 1000 mg/kg or female $B6C3F_1$ mice at doses of 250 or 500 mg/kg.
Method: NTP study
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance:Purity: > 99.5 %
Remarks:
Reference: US/NTP (1986)

5.8 TOXICITY TO REPRODUCTION

(a)
Type: Fertility **[ ]**; One generation study **[ ]**; Two generation study **[ ]**; Other **[X]**
Species/strain: Rat Crj:CD(SD)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Route of Administration: Oral (gavage)
Exposure period: Male: for 49 days including 14 days before mating
Female: 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, 2.4, 12, 60 or 300 mg/kg (12 /animals /sex/ group)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**;
Historical **[ ]**
NOEL Parental : < 2.4 mg/kg/day
NOEL F1 Offspring: 60 mg/kg/day
NOEL F2 Offspring: N/A
Results: As the effects to parents, the depression of body weight gain and 2 females death were observed in 300 mg/kg group. In the clinical observations, salivation was observed in all chemical treatment groups. Any change was not observed in gross and histopathological findings, and organ weights in males of each treatment group. Erosion and desquamation were seen on mucous in glandular stomach of 300 mg/kg females. The results observed in mating, fertility and estrous cycle did not reveal any effects attributable to the administration of the chemical. Observation of delivery, all gestation animals delivered of pups, normally and there were lack of care in behavior in 12 mg/kg group or more. The external examination of pups revealed depression of viability index and body weight gain in 300 mg/kg group.
Method: OECD/SIDS Preliminary Reproductive/Developmental Toxicity Screening Test
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Commercial, purity > 99.5 %
Remarks: None
Reference: MHW, Japan (1993a)

(b)
Type: Fertility **[ ]**; One generation study **[X]**; Two generation study **[ ]**; Other **[X]**
Species/strain: Rat (Wistar)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration: Oral (gavage)
Exposure period: First 19 days of pregnancy
Frequency of treatment:
Postexposure observation period:
Premating exposure period:
Duration of the test;
Doses: 0, 0.72, 110, 733 mg/kg
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**;
Historical **[ ]**
NOEL Parental : 110 mg/kg/day
NOEL F1 Offspring: 733 mg/kg/day
NOEL F2 Offspring: N/A
Results: An increase in embryo mortality was seen in the 733 mg/kg dose group; no effects were seen in the lower dose groups. There was an increase in the number of fetuses with internal organ hemorrhage in the 733 mg/kg dose group. Progeny of the dosed females were observed for 30 days following birth. No compound-related effects

were observed in mortality, body weight change, time of appearance of body hair, or opening of eyes. The offspring were crossbred (within dose group) and subsequently evaluated. Butyl chloride at a dose of 733 mg/kg substantially increased embryo mortality in the second generation. The author concluded that butyl chloride induced a hazardous effect on embryogenesis only in large doses that had pronounced toxic effects.

Method: Unknown
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance:
Remarks: None
Reference: Leonskaya, G. (1981)

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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