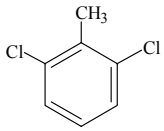
FOREWORD INTRODUCTION

2,6-DICHLOROTOLUENE

CAS N°: 118-69-4

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	118-69-4
Chemical Name	2,6-Dichlorotoluene
Structural formula	

CONCLUSIONS AND RECOMMENDATIONS

Environment

The chemical is not readily biodegradable and has relatively high bioconcentration potential. Although toxicity of the chemical seems relatively high to Daphnia, PEC/PNEC ratio is less than 1 based on the local exposure scenario in the Sponsor country. It is currently considered of low potential risk and low priority for further work.

Human health

The chemical is moderately toxic in a repeated dose study (i.e. liver, kidney, thymus) and reproductive/developmental toxicity study (maternal toxicity). Occupational exposure is expected to be low as it is produced in closed system in Sponsor country. No consumer use is reported. Estimated daily intake through indirect exposure is also considered to be low. As the margin of safety is more than 200, 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

2,6-Dichlorotoluene is stable liquid and the production volume is ca. 80 tonnes/year in 1996 in Japan. The chemical is used as intermediate for pesticide and pharmaceuticals. No consumer use is reported. The chemical is classified as “not readily biodegradable”. Bioconcentration factor is 246 – 828.

The potential environmental distribution of 2,6-dichlorotoluene obtained from a generic fugacity model (Mackey level III) showed the chemical would be distributed mainly to air and water. Predicted environmental concentration (PEC_{local}) of the chemical was estimated as 7.3×10^{-6} mg/l from Japanese local exposure scenario. In Japanese environmental survey, the chemical was not detected from surface water and sediments in 1982.

The main route of human exposure is inhalation with a limited numbers of workers potentially exposed during sampling operation. As there is no available data of the atmosphere concentration, the daily intake is calculated as 0.12 mg/kg/day as the worst case, based on the predicted high concentration and the possibility of exposure period. There is no available

information on consumer use. Indirect exposure via the environment, the daily intakes through drinking water and fish were estimated as 2.43 x 10^{-7} mg/kg/day and 9.07 x 10^{-6} mg/kg/day, respectively, based on PEC_{local} of 7.30 x 10^{-6} mg/l.

As the lowest acute and chronic toxicity data, 48 h EC50 (1.8 mg/l) value and 21 d NOEC (0.32 mg/l) of *Daphnia magna* were adopted, respectively. The assessment factors of 100 were used to both acute and chronic toxicity data to determine PNEC, because chronic toxicity data for fish was absent. Thus, PNEC of the chemical is 0.0032 mg/l. PEC/PNEC ratio is about 0.0023 and the bioconcentration factor of the chemical is moderate. Therefore, effects of the chemical on aquatic ecosystems are at low concern at present.

2,6-Dichlorotoluene had no genotoxic effects in bacteria and chromosomal aberration test *in vitro*. In a combined repeat dose and reproductive/developmental toxicity screening test, both male and female rats showed histopathological changes in liver, kidney and thymus, and maternal toxicity was observed. The no observed effect levels were obtained as 30 mg/kg/day for repeated dose toxicity and 100 mg/kg/day for reproductive toxicity.

For human health, the risk for workers is expected to be low because the margin of safety is 250. The risks for consumer and the general population through indirect exposure are also assumed to be low because the margin of safety through drinking water or fish is calculated to be 1.23 x 10^{8} or 3.31 x 10^{6}. Therefore, it is currently considered of low potential risk and low priority for further work.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE

FULL SIDS SUMMARY

CAS NO: 118-69-4		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		Unknown	2.8°C
2.2	Boiling Point		Unknown	199 - 200 °C
2.3	Density			
2.4	Vapour Pressure		OECD TG 104	34 Pa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	4.25 at 25 °C
2.6 A.	Water Solubility		OECD TG 105	26 mg/L at 25 °C
B.	pH			
	pKa			No ionizable functional Group
2.12	Oxidation: Reduction Potential			
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation			
3.1.2	Stability in Water		OECD TG 111	Stable at pH 4 and 7 at 25 °C 85.0 days at pH 9 at 25 °C
3.2	Monitoring Data			Surface water(sea) : ND Sediment(sea) : ND
3.3	Transport and Distribution			
3.5	Biodegradation		OECD TG 301C	Not readily biodegradable
3.7	Bioaccumulation	Carp	OECD TG 305C	BCF 381 – 567 at 0.02 m/L 246 – 828 at 0.002 mg/L
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oryzias latipes*	OECD TG 203	LC_{50}(48hr)= 7.9 mg/l LC_{50}(72hr)= 6.4 mg/l LC_{50}(96hr)= 6.4 mg/l
4.2	Acute Toxicity to Aquatic Invertebrates *Daphnia*	*Daphnia magna*	OECD TG 202	EC_{50}(48hr): 1.8 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD TG 201	EC_{50}(72hr) = 17.6 mg/l NOEC= 10 mg/l
4.5.2	Chronic Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50}(21d,Repro)= 0.47 mg/l NOEC= 0.32 mg/l
4.6.1	Toxicity to Soil Dwelling Organisms			None
4.6.2	Toxicity to Terrestrial Plants			None
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)			None

TOXICOLOGY				
5.1.1	Acute Oral Toxicity			No data
5.1.2	Acute Inhalation Toxicity			No data
5.1.3	Acute Dermal Toxicity			No data
5.4	Repeated Dose Toxicity	Rat	OECD Combined	NOEL = 30 mg/kg
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	S. typhimurium E. coli WP2	Japanese TG	- (With metabolic activation) - (Without metabolic activation)
B.	Non-Bacterial In Vitro Test (Chromosomal aberrations)	Chinese hamster CHL cells	Japanese TG	- (With metabolic activation) - (Without metabolic activation)
5.6	Genetic Toxicity In Vivo			No data
5.8	Toxicity to Reproduction	Rat	OECD combined	NOEL = 100 mg/kg
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
for
8th SIAM
(France, October 28-30, 1998)

Chemical Name: 2,6-Dichlorotoluene
CAS No: 118-69-4
Sponsor Country: Japan

National SIDS Contact Point in Sponsor Country:
Mr. Kenichi Suganuma
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
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

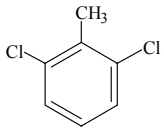
Deadline for circulation: July 31, 1998
Date of Circulation: October 5, 1998
(To all National SIDS Contact Points and the OECD Secretariat)

SIDS INITIAL ASSESSMENT REPORT

2,6-Dichlorotoluene
(CAS No. 118-69-4)

1. IDENTITY

- OECD Name: 2,6-Dichlorotoluene
- Synonym: Benzene, 1,3-dichloro-2-methyl-
- CAS Number: 118-69-4
- Empirical Formula: $C_7H_6Cl_2$
- Structural Formula:



- Degree of Purity: 99 %
- Major Impurity: 2,5-Dichlorotoluene, 2,3-Dichlorotoluene, 2,4-Dichlorotoluene
- Essential Additives: None
- Physical-chemical properties
  - Melting Point: 2.8 °C
  - Vapour pressure: 34 Pa at 25 °C
  - Water solubility: 26 mg/L
  - Log Pow: 4.25

2. GENERAL INFORMATION ON EXPOSURE

2.1 Production and import

80 tonnes/year in 1996 in Japan

2.2 Use pattern

Intermediate in closed system.

Intermediate for pesticides and pharmaceuticals

2.3 Other information

3. ENVIRONMENT

3.1 Environmental Exposure

3.1.1 General Discussion

2,6-dichlorotoluene is not readily biodegradable (OECD 301C: 0% after 28d) and stable in water. Direct photodegradation could be expected because 2,6-dichlorotoluene has absorption band in UV region.

2,6-dichlorotoluene is moderately bioaccumulative based on the test using carp (OECD 305C: BCF 380 – 570 at 0.02 mg/l).

The potential environmental distribution of 2,6-dichlorotoluene obtain from generic Mackay level III fugacity model is shown in Table 1. Parameters used for this model is shown as Annex to this report. The results show that, if 2,6-dichlorotoluene is released into air or soil, it is unlikely to be distributed into other compartment. If 2,6-dichlorotoluene is released into water, it is likely to be transported to air.

Table 1 Environmental distribution of 2,6-dichlorotoluene Using a generic level III fugacity model.

Compartment	Release 100% to air	Release 100% to water	Release 100% to soil
Air	89.8 %	24.4 %	0.2 %
Water	1.7 %	63.9 %	0.0 %
Soil	8.3 %	2.2 %	99.8 %
Sediment	0.3 %	9.4 %	0.0 %

As this chemical is used in closed systems as an intermediate and is not included in consumer products, its release to the environments may occur only from the production cites.

3.1.2 Predicted Environmental Concentration

As 2,6-dichlorotoluene is produced under the well controlled closed systems, amount of release to air phase is negligibly small. The waste of 2,6-dichlorotoluene from the production system is released to water phase after treated through its own waste-water treatment plant. Therefore, Predicted Environmental Concentration (PEC) will be calculated only for the water environment.

a. Local exposure

According to the report from a manufacturer in Japan, 72 kg/year (measured) of 2,6-dichlorotoluene was released with 3.4 x 1010 L/year of effluent into a bay in 1994. Local Predicted Environmental Concentration (PEClocal) is calculated to be 7.3 x 10-6 mg/L, employing the following calculation model and dilution factor of 290 (See Appendix 1).

Amount of release (7.2 x 107 mg/y)
Volume of effluent (3.4 x 1010 L/y) x Dilution Factor (290)

3.2 Effects on the Environments

3.2.1 Effects on aquatic organisms

Acute and chronic toxicity data of 2,6-Dichlorotoluene to aquatic organisms are summarized below (Table 2). Toxicity of this chemical seems relatively high to Daphnia. Predicted No Effect Concentration (PNEC) of this chemical was determined based on the toxicity data obtained by the

Environment Agency of Japan, because other data by different organizations were not available in the AQUIRE and IUCLID. As the lowest acute and chronic toxicity data, 48 h EC50 (immobility) value and 21 d NOEC (reproduction) of Daphnia magna were adopted, respectively (Table 2). The assessment factors of 100 were used to both acute and 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 acute toxicity data (48 h EC50 of Daphnia): PNEC = 1.8/ 100 = 0.018 mg/l
From chronic toxicity data (21 d NOEC of Daphnia): PNEC = 0.32/ 100 = 0.0032 mg/l

Thus, PNEC of 2,6-Dichlorotoluene is 0.0032 mg/l.

Table 2 Acute and chronic toxicity data of 2,6-Dichlorotoluene to aquatic organisms at different trophic levels. The data were obtained by the Environmental Agency of Japan based on the OECD Test Guide Lines.

Species	Endpoint	Conc. (mg/l)	Remarks
Selenastrum capricornutum (algae)	Gro 72 h EC50	17.6	a, 1), A
	do. 72 h NOEC	10.0	c, 1), C
Daphnia magna (Water flea)	Imm 24 h EC50	1.8	a, 1), A
	Rep 21 d EC50	0.47	c, 1)
	Rep 21 d NOEC	0.32	c, 1), C
Oryzias latipes (fish, Medaka)	Mor 1 d LC50	10.0	a, 1)
	Mor 2 d LC50	7.9	a, 1)
	Mor 3 d LC50	6.4	a, 1)
	Mor 4 d LC50	6.4	a, 1), A

Notes: Gro; growth, Mor; mortality, Rep; reproduction,
No. 1, reference number, A), C); the lowest values among the acute or chronic toxicity data of algae, cladocera (water flea) and fishes to determine PNEC of 2,6-Dichlorotoluene.

References

1) Toxicity data of the tests were conducted by the Environment Agency of Japan based on OECD Test Guide Lines.

3.2.2 Terrestrial effects

No data available

3.2.3 Other effects

No data available

3.3 Initial Assessment for the Environment

Predicted No Effect Concentration (PNEC) of this chemical has been calculated as 0.0032 mg/l. PEC from Japanese local exposure scenario is 7.3×10^{-6} mg/l.

$$PEClocal / PNEC = 7.3 \times 10^{-6} / 0.0032 = 0.0023 < 1$$

Therefore, it is currently considered of low potential risk for environments and low priority for further work.

4. HUMAN HEALTH

4. 1 Human Exposure

4. 1. 1 Occupational exposure

2,6-Dichlorotoluene is produced in closed systems and the occupational exposures in production sites were expected by inhalation during sampling operation. As the atmosphere concentration has not been measured, the exposure levels were estimated by the following information, using EASE model. Duration and frequency of sampling operation are 1 minute and 8 times/day. The concentrations in atmosphere are estimated in range of 10 to 50 mg/m^3. Workers wear protective gloves and respiratory protective equipment (mask) during the operation. If a single worker (body weight; 70 kg, respiratory volume; 1.25 m^3/hour) is assigned to implement all daily operation without protection equipment, the daily intake is calculated in range of 0.024 to 0.12 mg/kg/day as the worst cases.

4. 1. 2 Consumer exposure

There are no available data.

4. 1. 3 Indirect exposure via the environment

As 2,6-dichlorotoluene is persistent in water and bioaccumulative, the exposure to the general population via the environment would be possible through drinking water processed from surface water and through fish which may accumulate this chemical.

The concentration in drinking water should be estimated to be equal to PEC calculated in Section 3.1, i.e. 7.30 x 10^{-6} mg/l. The daily intake through drinking water is calculated as 2.43 x 10^{-7} mg/kg/day (2 l/day, 60 kg b.w.).

Using the maximum bioconcentration factor of 828 obtained by tests, the concentration of this chemical in fish can be calculated as follows:

$$PEC_{fish} = (7.30 \times 10^{-6} \text{ mg/l}) \times 828 = 6.04 \times 10^{-6} \text{ mg/g-wet}$$

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 9.07 x 10^{-6} mg/kg/day.

4. 2 Effects on Human Health

a) Acute toxicity
There are no available data. However, oral LD_{50} value of 2,6-dichlorotoluene could be expected to be at least more than 1000 mg/kg/day because all of male and female SD rats survived in an OECD combined repeat dose and reproductive/developmental toxicity screening test at 1000 mg/kg/day as described below. In addition, oral LD_{50} values of 2,4-dichlorotoluene, a structurally related chemical, are more than 2000 mg/kg for male and female SD rats.

b) Irritation
There are no available data.

c) Sensitisation
There are no available data.

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 at doses of 0 (vehicle; corn oil), 30, 100, 300, 1000 mg/kg/day.

Decrease in locomotor activity, reduction of body weight gain and increase in relative weight of liver and kidney were observed at 300, 1000 mg/kg in male and 1000 mg/kg in female. In the histopathological examination, hypertrophy and ground glass appearance of hepatocyte (at 300 and 1000 mg/kg), increase of eosinophilic body in kidneys (at 100, 300 and 1000 mg/kg) were observed in male rats. In female rats, hypertrophy of hepatocyte, degeneration of proximal tubule in kidney and atrophy of thymus were observed at 300 and 1000 mg/kg. In biochemical, hematological and urinalysis findings, no toxic effects were observed. NOEL was considered to be 30 mg/kg/day for male and 100 mg/kg/day for female, respectively.

e) Reproductive/developmental toxicity
[SIDS data] Oral toxicity study was performed in SD (Crj:CD) rats by an OECD combined repeated dose and reproductive/developmental toxicity screening test at doses of 0 (vehicle; corn oil), 30, 100, 300, 1000 mg/kg.

The number of implantation in 2 dams at 1000 mg/kg was markedly decreased to 2 or 3 from the average number of 16. One of them was delivered of a stillborn offspring, and another dam was delivered of a live offspring, which died up to day 4 after birth. The viability on day 4 after birth decreased at 300 and 1000 mg/kg. Especially, a dam at 300 mg/kg lost all of 14 offsprings up to day 4 after birth and a dam at 1000 mg/kg lost four of 17 offsprings up to day 4 after birth. It was considered that these changes might occur as a result of abnormal nursing, which was observed in some dams at 300 and 1000 mg/kg. As for offsprings, the decrease in body weight on day 4 of lactation was observed at 1000 mg/kg. But this change was not significant compared to the control. There were no other toxic changes and birth index including morphological findings. NOELs for female parents and offsprings were considered as 100 mg/kg and 300 mg/kg, based on reduction of implantation number, decrease in the viability on day 4 after birth, abnormal nursing, and weight change, respectively. The male reproductive toxicity might not occur under these conditions.

f) Genetic toxicity
[SIDS data] Gene reverse mutation was negative in *S. Typhimurium* TA100, TA98, TA1535, TA1537 and *E.coli* WP2 *uvr*A with and without metabolic activation. Structural chromosomal aberration or polyploidy in CHL/IU cells were not induced up to the concentration, at which cytotoxicity was observed, in the absence or presence of an exogenous metabolic activation system.

4.3 Initial Assessment for Human Health

2,6-Dichlorotoluene was not mutagenic in bacterial test and chromosomal aberration test in vitro. In a combined repeat dose and reproductive/developmental toxicity study, histopathological changes in liver, kidney and thymus, and reproductive toxicity were observed. NOELs were 30 mg/kg/day for repeated dose toxicity and 100 mg/kg/day for reproductive toxicity.

2,6-Dichlorotoluene is used a closed system at industries and workers wear protective gloves and respiratory protective equipment during the sampling operation. As the exposure route for human may be an inhalation in limited workers, there is no available data of the atmosphere concentration. Based on the predicted high concentration and the possibility of exposure period, the daily intake is calculated as 0.12 mg/kg/day as the worst case. Occupational risk is presumably low because the margin of safety is 250. There is no available information on consumer use.

As for indirect exposure via environment, PEC_{local} of 7.30 x 10^{-6} mg/l from local exposure scenario was used for the estimation. The daily intakes through drinking water and fish are calculated as 2.43 x 10^{-7} mg/kg/day and 9.07 x 10^{-6} mg/kg/day, respectively. Since the margin of safety is very large, such as 1.23 x 10^{8} for drinking water and 3.31 x 10^{6} for fish, health risk is presumably low.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

2,6-Dichlorotoluene is not readily biodegradable and has relatively high bioconcentration potential. Although toxicity of the chemical seems relatively high to Daphnia, PEC/PNEC ratio is less than 1 based on the local exposure scenario in the Sponsor country. It is currently considered of low potential risk and low priority for further work.

2,6-Dichlorotoluene is moderately toxic in a repeated dose study (i.e. liver, kidney, thymus) and reproductive/developmental toxicity study (maternal toxicity). Occupational risk is expected to be low because of low predicted daily intake from the atmosphere in the production sites. The estimated daily intake through indirect exposure is also considered to be low. As the margin of safety is very large, it is currently considered of low potential human risk and low priority for further work.

5.2 Recommendations

No recommendation

6. REFERENCES

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.

$$PEC_{local}\ (mg/L) = \frac{Co\ Q + Cs\ Qs}{Q + Qs} \quad (1)$$

Where
Co: Concentration of pollutant in upper stream of release point (mg/L)
Cs: Concentration of pollutant in effluent (mg/L)
Q : Flow rate of river(m^3/day)
Qs: Flow rate of effluent released into river(m^3/ day)

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

$$R = Cs/C = (Q + Qs) / Qs \quad (2)$$

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-Sendner 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.

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

Where
C(x): Concentration of pollutant at distance x(m) from release point
Cs : Concentration of pollutant in effluent
C(r) : Concentration of pollutant at distance r(m) from release point
Qs : 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=∞ and density stratification is ignored for simplification, Joseph-Sendner equation(4) is simplified to equation(5)

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

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

$$R(x) = C_s/C(x) = \theta\, d\, p\, x/Q_s \qquad (6)$$

When it is employed following parameters in equation (6) as default, dilution factor R can be shown with equation (7).
P = 1 cm/sec(860m/day)
θ = 3.14
d = 10m
x = 1000m

$$R = 2.7 \times 10^7/Q_s \qquad (7)$$

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

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE 4 CHEMICAL

2,6-Dichlorotoluene

CAS No. 118 - 69 -4

Sponsor Country: Japan
Date: October 5, 1998

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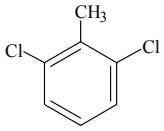
6. REFERENCES

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

S I D S P R O F I L E
DATE: October 5, 1998

1.01 A.	**CAS No.**	118-69-4
1.01 C.	**CHEMICAL NAME (OECD Name)**	2,6-Dichlorotoluene
1.01 D.	**CAS DESCRIPTOR**	
1.01 G.	**STRUCTURAL FORMULA**	
	OTHER CHEMICAL IDENTITY INFORMATION	
1.5	**QUANTITY**	80 tonnes/year in 1996 in Japan
1.7	**USE PATTERN**	Intermediate, Intermediate in closed system, Intermediate for pesticides and pharmaceuticals.
1.9	**SOURCES AND LEVELS OF EXPOSURE**	72 kg/year Release into a bay
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)	SIDS testing required: Water solubility Octanol/water partition coefficient Stability in water Acute toxicity to fish, daphnia and algae Chronic toxicity to daphnia Combined repeat dose and developmental toxicity Gene mutation Chromosomal aberration in vitro	

S I D S S U M M A R Y

DATE: October 5, 1998

CAS NO: 118-69-4		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	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
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	Y	N	N	Y	N	Y	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	N						N
5.1.2	Acute Inhalation	N						N
5.1.3	Acute Dermal	N						N
5.4	Repeated Dose	N						Y
5.5	Genetic Toxicity *in vitro*							
	. Gene mutation	N						Y
	. Chromosomal aberration	N						Y
5.6	Genetic Toxicity *in vivo*	N						N
5.8	Reproduction Toxicity	N						Y
5.9	Development / Teratogenicity	N						N
5.11	Human experience	N						N
OTHER TOXICITY STUDIES RECEIVED								

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

***A. CAS number** 118-69-4

B. Name *(IUPAC name)*

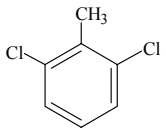
***C. Name** *(OECD name)* 2,6-Dichlorotoluene

†D. CAS Descriptor

E. EINECS-Number 204-269-7

F. Molecular Formula $C_7H_6Cl_2$

***G. Structural Formula**



H. Substance Group

I. Substance Remark

J. Molecular Weight 161.03

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. kenichi Suganuma
Director, Second International Organization Bureau
Ministry of Foreign Affairs

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

C. Name of responder

Name: Same as above contact person

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 **[X]**; solid **[ ]**

C. Purity 99%

1.2 SYNONYMS

Benzene, 1,3-dichloro-2-methyl-

1.3 IMPURITIES

Name: 2,5-Dichlorotoluene, 2,3-Dichlorotoluene, 2,4-Dichlorotoluene

1.4 ADDITIVES

None

*1.5 QUANTITY

Remarks: 80 tonnes/year in 1996
Reference: MITI, Japan

1.6 LABELLING AND CLASSIFICATION

*1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Intermediate
industrial	Intermediate in closed system
use	Intermediate for pesticide and Pharmaceuticals

Remarks: None
Reference: MITI

1.8 OCCUPATIONAL EXPOSURE LIMIT

None

* 1.9 SOURCES OF EXPOSURE

In Japan, 2,6-dichlorotoluene is produced by 1 company.

Source: Media of release:. Bay
Quantities per media: 72kg/year in 1994 (measured)
Remarks:
Reference: MITI, Japan

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: 2.8°C
Decomposition: Yes [ ] No [X] Ambiguous [ ]
Sublimation: Yes [ ] No [X] Ambiguous [ ]
Method:
GLP: Yes [ ] No [X] ? [ ]
Remarks:
Reference: KAGAKU DAIJITENN

*2.2 BOILING POINT

Value: 199 - 200 °C
Pressure: at 1.013 hPa
Decomposition: Yes [ ] No [X] Ambiguous [ ]
Method:
GLP: Yes [ ] No [X] ? [ ]
Remarks:
Reference: KAGAKU DAIJITENN

*2.4 VAPOUR PRESSURE

Value: 34 Pa
Temperature: 25 °C
Method: calculated [ ]; measured [X]
GLP: Yes [X] No [ ] ? [ ]
Remarks:
Reference: MITI, JAPAN.

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

Log Pow: 4.25
Temperature: 25 °C
Method: calculated [ ]; measured [X]
OECD TG 107
GLP: Yes [X] No [ ] ? [ ]
Remarks:
Reference: MITI, JAPAN.

***2.6 WATER SOLUBILITY**

A. Solubility

Value:	26 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 TG 105
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
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:	Stable at pH 4 at 25 °C Stable at pH 7 at 25 °C 85.0 days at pH 9 at 25 °C
Method:	OECD TG 111
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	2,6-Dichlorotoluene, purity: 99%
Remarks:	
Reference:	MITI, JAPAN.

*3.2 MONITORING DATA (ENVIRONMENTAL)

(a)

Type of Measurement:	Background **[ ]**; At contaminated site **[ ]**; Other **[x]**
Media:	Surface water (sea)
Results:	ND (Detection limits: 0.08 – 0.008 mg/l) in 7 areas in Japan as of 1981
Remarks:	ND: Not detected
Reference:	Chemicals in the environment, EA, Japan (1982)

(b)

Type of Measurement:	Background **[ ]**; At contaminated site **[ ]**; Other **[x]**
Media:	Sediment (sea)
Results:	ND (Detection limits: 0.20 mg/kg-dry) in 7 areas in Japan as of 1981
Remarks:	ND: Not detected
Reference:	Chemicals in the environment, EA, Japan (1982)

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	89.8 %	24.4 %	0.2 %
Water	1.7 %	63.9 %	0.0 %
Soil	8.3 %	2.2 %	99.8 %
Sediment	0.3 %	9.4 %	0.0 %

Remarks: Appendix 1

*3.5 BIODEGRADATION

Type: aerobic **[X]**; anaerobic **[ ]**
Inoculum: adapted **[ ]**; non-adapted **[X]**;
Concentration of the chemical: related to COD **[ ]**; DOC **[ ]**; test substance **[X]**
Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation: 0 % after 28 days
Results: readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[X]**, other **[ ]**
Method: OECD TG 301C .
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: 2,6-dichlorotoluene , purity: 99%
Reference: MITI, JAPAN.

3.7 BIOACCUMULATION

Species: Carp (*Cyprinus carpio*)
Exposure period: 8 weeks
Temperature: 25 °C
Concentration: (1) 0.02 m/L
(2) 0.002 mg/L
BCF: (1) 381 – 567
(2) 246 – 828
Method: OECD TG 305C
Type of test: calculated **[ ]**; measured **[x]**
static **[ ]**; semi-static **[ ]**; flow-through **[x]**; other *(e.g. field test)* **[ ]**
GLP: Yes **[x]** No **[ ]** ? **[ ]**
Test substance: 2,6-Dichlorotoluene, purity: 99 %

Remarks:
Reference: MITI, JAPAN.

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test:	static [ ]; semi-static [X]; flow-through [ ]; other (e.g. field test) [ ] open-system [X]; closed-system [ ]
Species:	*Oryzias latipes* (Himedaka)
Exposure period:	96 h
Results:	LC50 (24h) = 10 mg/l LC50 (48h) = 7.9 mg/l LC50 (72h) = 6.4 mg/l LC50 (96h) = 6.4 mg/l
Analytical monitoring:	Yes [ ] No [X] ? [ ]
Method:	OECD TG 203 (1992)
GLP:	Yes [ ] No [X] ? [ ]
Test substance:	As prescribed by 1.1 - 1.4, purity: >98%
Remarks:	Group of ten Himedaka were exposed to nominal concentrations of 1.7, 3.1, 5.6, 10 and 18 mg/l, DMSO (550 µg/l) control and laboratory water control. The LC50 (96h) was determined to be 6.4 mg/l with a 95 % confidence level (5.6 mg/l to 7.8 mg/l).
Reference:	Environment Agency of JAPAN (1994)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*A. Daphnia

Type of test:	static [ ]; semi-static [X]; flow-through [ ]; other (e.g. field test) [ ]; open-system [X]; closed-system [ ]
Species:	*Daphnia Magna.*
Exposure period:	24 h
Results:	EC50 (48h) = 1.8 mg/l NOEC = 1.2 mg/l
Analytical monitoring:	Yes [ ] No [X] ? [ ]
Method:	OECD TG 202 .
GLP:	Yes [ ] No [X] ? [ ]
Test substance:	As prescribed by 1.1 - 1.4, purity: >98%
Remarks:	20 daphnids (4 replicates; 5 organisms per replicate) were exposed to nominal concentrations of 1, 1.2, 1.4, 1.7 and 2.0 mg/l, solubilizer (Tween 80, 0-55 mg/l) control and laboratory water control. The EC50 (24h) was determined to be 1.8 mg/l with a 95 % confidence level of 1.7 mg/l to 1.9 mg/l.
Reference:	Environment Agency of JAPAN (1994).

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

Species:	*Selenastrum capricornutum* ATCC 22662	
Endpoint:	Biomass [X]; Growth rate [ ]; Other [ ]	
Exposure period:	72 h	
Results:	Biomass	EC50 (72h) = 17.6 mg/l NOEC = 10 mg/l
Analytical monitoring:	Yes [X] No [ ] ? [ ]	
Method:	OECD TG 201 (1984) open-system [ ]; closed-system [X]	
GLP:	Yes [ ] No [X] ? [ ]	
Test substance:	purity: >98%	
Remarks:	Static test. The EC50 value for growth rate (% inhibition) was calculated based on 5 nominal concentrations (1.5, 2.8, 5.0, 9.0 and 16 mg/l) . Minimal amount of Tween 80 – acetone (1:1) or DMSO - HCO-40 (9:1) is used as solubilizer.	
Reference:	Environment Agency of JAPAN (1994)	

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 [ ]; semi-static [X]; flow-through [ ]; other (e.g. field test) [ ]; open-system [X]; closed-system [ ]	
Species:	*Daphnia Magna*	
Endpoint:	Mortality [ ]; Reproduction rate [X]; Other [X]	
Exposure period:	21 d	
Results:	Reproduction rate:	EC50 (21 d) = 0.47 mg/l NOEC = 0.32 mg/l LOEC = 0.56 mg/l
	Immobility:	EC50(48h) = 2.0 mg/l EC50 (21 d) = 0.47 mg/l
Analytical monitoring:	Yes [ ] No [X] ? [ ]	
Method:	OECD TG 202(1984)	
GLP:	Yes [ ] No [X] ? [ ]	
Test substance:	As prescribed by 1.1 - 1.4, purity: >98%	
Remarks:	40 daphnids (4 replications of 10 daphnids in a 500 ml beaker) were exposed to 5 concentrations (0.18, 0.32, 0.56, 1.0, 1.8 mg/l) in dechlorinated tap water (pH: 7.6 to 8.0; Hardness : 46 to 250 mg/l). A mixture of DMSO and HCO-40 (4:1) was used as a solubilizer. 1.8-18 mg/l of the mixture was added to the dechlorinated tap water to prepare the nominal concentrations.	

Reference: Environment Agency of JAPAN (1994).

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

There are no available data.

[2,4-Dichlorotoluene: a structurally related chemical]
Type: LD_0 [ ]; LD_{100} [ ]; LD_{50} [X]; LDL_0 [ ]; Other [ ]
Species/strain: Rat/Crj:CD
Value: :>2000 mg/kg for male and female
Discriminating dose: 500, 1000, 2000 mg/kg
Method: OECD Test Guideline 401
GLP: Yes [X] No [ ] ? [ ]
Test substance: 2,4-dichlorotoluene, purity: 98.96%
Remarks:
Reference: MHW Japan (1994)

5.1.2 ACUTE INHALATION TOXICITY

No data

5.1.3 ACUTE DERMAL TOXICITY

No data

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

No data

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

No data

5.2.2 EYE IRRITATION/CORROSION

No data

5.3 SKIN SENSITISATION

No data

*5.4 REPEATED DOSE TOXICITY (SIDS data)

Species/strain:	Rats/Cij;CD (SD)
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration:	Oral (by gavage)
Exposure period:	For 2 weeks prior to mating and 2 weeks of mating. Further for 2 weeks after mating in males and throughout pregnancy up till day 3 post partum in females.
Frequency of treatment:	Daily
Post exposure observation period:	1 day
Dose:	30, 100, 300, 1000 mg/kg/day (in corn oil)
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL:	Male: 30 mg/kg/day Female: 100 mg/kg/day
LOEL:	Male: 100 mg/kg/day Female: 300 mg/kg/day
Results:	Decrease in locomotor activity, reduction of body weight gain and increase in relative weight of liver and kidney were observed at 300, 1000 mg/kg in male and 1000 mg/kg in female. In the histopathological examination, hypertrophy and ground glass appearance of hepatocyte (at 300 and 1000 mg/kg), increase of eosinophilic body in kidneys (at 100, 300 and 1000 mg/kg) were observed in male rats. In female rats, hypertrophy of hepatocyte, degeneration of proximal tubule in kidney and atrophy of thymus were

observed at 300 and 1000 mg/kg. In biochemical, hematological and urinalysis findings, no toxic effects were observed.

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

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

Test substance: purity: 99.2 %

Reference: MHW, Japan (1997)

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: Bacterial reverse mutation assay

System of testing: *Salmonella typhimurium* TA100, TA1535, TA98, TA1537
Escherichia coli WP2 uvrA

Concentration: -S9: 0, 2.344, 4.688, 9.375, 18.75, 37.5, 75 and 150 mg/plate (TA1535), 0, 4.688, 9.375, 18.75, 37.5, 75 and 150 mg/plate (TA100, TA98, TA1537, WP2)
+S9: 0, 9.375, 18.75, 37.5, 75, 150, 300 and 600 mg/plate (TA1535), 0, 18.75, 37.5, 75, 150, 300 and 600 mg/plate (TA100, TA98, TA1537, WP2)

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**

S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone.

Results:

Cytotoxicity conc: as results of preliminary cytotoxicity test

With metabolic activation: >500 μg/plate (TA100, TA98, TA1537, WP2), >150 μg/plate (TA1535)

Without metabolic activation: >150 μg/plate (TA100, TA98, TA1537, WP2), >50 μg/plate (TA1535)

Precipitation conc:

Genotoxic effects:

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

Method: Guidelines for Screening Mutagenicity Testing of Chemicals Japan, and OECD TG (471 and 472)

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

Test substance: 2,6-Dichlorotoluene, purity: 99.6 %

Remarks:

Reference: MHW, Japan (1997)

B. NON-BACTERIAL IN VITRO TEST

Type: Chromosomal aberration test

System of testing: CHL/IU cell

Concentration: -S9 (continuous treatment): 0, 0.017, 0.035, 0.069 mg/ml
-S9 (short-term treatment): 0, 0.008, 0.017, 0.033 mg/ml
+S9 (short-term treatment): 0, 0.024, 0.048, 0.096 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: Without metabolic activation: 0.096 mg/ml
Without metabolic activation: 0.069 mg/ml (continuous treatment), 0.033 mg/ml (short-term treatment)
Precipitation conc:
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [X]**
Without metabolic activation: **[ ] [ ] [X]**
Method: Guide for Screening Mutagenicity Testing of Chemicals (Japan), and OECD TG (473).
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: 2,6-Dichlorotoluene, purity: 99.6 %
Remarks:
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: For 2 weeks prior to mating, 2 weeks of mating and 2 weeks after mating.
Female: For 2 weeks prior to mating, 2 weeks of mating and throughout pregnancy up till day 3 postarm.
Frequency of treatment: Daily
Post exposure observation period: 1 day
Premating exposure period: male: 14 days, female: 14 days
Duration of the test:
Dose: 30, 100, 300, 1000 mg/kg/day (in corn oil)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**; Corn oil
Concurrent no treatment **[ ]**; Concurrent vehicle **[X]**; Historical **[ ]**
NOEL Parental: Male; 1000 mg/kg, Female; 100 mg/kg
NOEL F1 Offspring: 300 mg/kg
NOEL F2 Offspring:
Results:

General parental toxicity:

The number of implantation decreased markedly in 2 dams at 1000 mg/kg. One of them was delivered of a stillborn offspring and another dam was delivered of a live offspring, which died up to day 4 after

birth. The viability on day 4 after birth decreased at 300 and 1000 mg/kg. Especially, a dam at 300 mg/kg lost all of 14 offsprings up to day 4 after birth and a dam at 1000 mg/kg lost four of 17 offsprings up to day 4 after birth. It was considered that these changes might occur as a result of abnormal nursing, which was observed in some dams at 300 and 1000 mg/kg. In male rats no reproductive toxicity were observed.

Toxicity to offspring:

The decrease in body weight on day 4 of lactation was observed at 1000 mg/kg. But this change was not significant compared to the control. In morphological findings, no change was observed.

Method: OECD Combined Repeat Dose and Reproductive Toxicity Screening Test
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: purity: 99.2 %
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 available data

6. REFERENCES

MHW, Japan (1997)

Appendix 1

2,6-Dichlorotoluene

scenario 1

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	1,000	8.9.E-06	8.9.E+04	89.8	1.1E+02	8.9.E+02
water	0	8.5.E-05	1.7.E+03	1.7	2.7E-01	1.7.E+00
soil	0	5.1.E-03	8.1.E+03	8.3	1.3E+00	
sediment		2.5.E-03	2.5.E+02	0.3	4.0E-02	5.0.E-03
		total amount	9.9.E+04			

scenario 2

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	0	7.0.E-06	7.0.E+04	24.4	8.8.E+01	7.0.E+02
water	1000	9.1.E-03	1.8.E+05	63.9	2.9.E+01	1.8.E+02
soil	0	4.0.E-03	6.4.E+03	2.2	1.0.E+00	
sediment		2.7.E-01	2.7.E+04	9.4	4.3.E+00	5.4.E-01
		total amount	2.9.E+05			

scenario 3

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	0	1.2.E-06	1.2.E+04	0.2	1.5.E+01	1.2.E+02
water	0	5.1.E-05	1.0.E+03	0.0	1.6.E-01	1.0.E+00
soil	1000	3.4.E+00	5.4.E+06	99.8	8.6.E+02	
sediment		1.5.E-03	1.5.E+02	0.0	2.4.E-02	3.0.E-03
		total amount	5.4.E+06			

scenario 4

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	600	7.5.E-06	7.5.E+04	11.0	9.5.E+01	7.5.E+02
water	300	2.8.E-03	5.6.E+04	8.1	9.0.E+00	5.6.E+01
soil	100	3.4.E-01	5.5.E+05	79.7	8.8.E+01	
sediment		8.2.E-02	8.2.E+03	1.2	1.3.E+00	1.6.E-01
		total amount	6.8.E+05			

Physico-chemical parameter

molecular weight		161.03	Measured
melting point °C		2.8	Measured
vapor pressure [Pa]		3.40E+01	Measured
water solubility [g/m^3]		26	Measured
log Kow		4.25	Measured
half life [h]	in air	550	Estimated
	in water	4320	Estimated
	in soil	4320	Estimated
	in sediment	4320	Estimated

Temp. [°C]	25

Environmental parameter

		volume	depth	area	organic	lipid content	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 : 522711
!!! WARNING - not original IRPTC record - WARNING !!!
reported name :2,6-Dichlorotoluene
cas no :118-69-4
area : DEU type : REG

subject	specification	descriptor
AQ USE	INDST	CLASS RQR

This substance is classified as hazardous to water (Water Hazard Class: WHC 2). (There are 3 water hazard classes: WHC 3 = severely hazardous; WHC 2 = hazardous; WHC 1 = moderately hazardous; and the classification as "not hazardous to water"). The purpose of the classification is to identify the technical requirements of industrial plants which handle substances hazardous to water.
entry date: SEP 2001 effective date: 01JUN1999

title: Administrative Order relating to Substances Hazardous to Water (Verwaltungsvorschrift wassergefaehrdende Stoffe)
original : BUANZ*, Bundesanzeiger, 51 , 98a , 1 , 1999

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file: 17.01 LEGAL rn : 1470485
!!! WARNING - not original IRPTC record - WARNING !!!
reported name :2,6-Dichlorotoluene
cas no :118-69-4
area : EEC type : REG

subject	specification	descriptor
MANUF	INDST	CLASS
IMPRT	INDST	CLASS

The substance is included in a list of existing substances produced or imported within the Community in quantities exceeding 1000 tonnes per year. - A system of data reporting by any manufacturer who has produced or any importer who has imported the substance, as such or in a preparation, in quanities exceeding 10 tonnes per year is established.
entry date: AUG 1999 effective date: 04JUN1993

title: Council Regulation (EEC) No 793/93 of 23 March 1993 on the evaluation and control of the risks of existing substances
original : OJECFC, Official Journal of the European Communities, L84 , , 1 , 1993