FOREWORD INTRODUCTION

DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE

CAS N°: 840-65-3

SIDS Initial Assessment Report
for
9th SIAM
(France, June 29-July 1, 1999)

Chemical Name: Dimethyl 2,6-naphthalenedicarboxylate
CAS No: 840-65-3
Sponsor Country: Japan

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

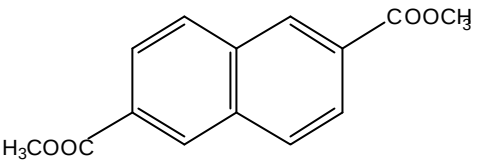
HISTORY:

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

no testing ( )
testing (X) Water solubility, Vapour pressure, Octanol/water partition coefficient
Stability in water, Biodegradation
Chronic toxicity to daphnia
Acute toxicity, Combined repeat dose and reproductive toxicity
Gene mutation, Chromosomal aberration test in vitro

Deadline for circulation: March 31, 1999
Date of Circulation: March 30, 1999
(To all National SIDS Contact Points and the OECD Secretariat)

SIDS INITIAL ASSESSMENT PROFILE

CAS NO.	840-65-3
CHEMICAL NAME	Dimethyl 2,6-naphthalenedicarboxylate
Structural formula	

RECOMMENDATIONS OF THE SPONSOR COUNTRY

The chemical is currently of low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE RECOMMENDATIONS

Dimethyl 2,6-naphthalenedicarboxylate is stable in water ($T_{1/2}$ = 263 days at pH 7 at 25°C). This chemical is not readily biodegradable (OECD 301 C: 7% after 28-day) and moderately bioaccumulative (BCF in Carp = 6.1~63).

No toxicity was observed up to the maximum dispersible concentration with a dispersant (THF/HCO-30). For testings in algae, *Selenastrum capricornutum* (72-h EC_{50}, 72-h NOEC), in fish, Medaka (96-h LC_{50}, 14-day LC_{50} of *Oryzias latipes*), and in daphnid, *Daphnia magna* (24-h EC_{50} for immobilisation), all results were more than 0.1 mg/l, which is the highest concentration that this chemical can be dispersed. For the daphnid reproduction test, 24-h EC_{50} was 0.02 mg/l, which was also the maximum dispersible concentration using a different dispersant (TMF/HCO-50).

Oral LD_{50} of this chemical for rats is more than 2,000 mg/kg. There are no available data for irritation and sensitisation. In an OECD combined repeat dose and reproductive/developmental toxicity study in rats at 30, 100, 300 and 1000 mg/kg/day, no toxic effects were observed. Therefore, NOAEL was considered to be 1000 mg/kg/day for both repeated dose toxicity and reproductive toxicity. This chemical is not genotoxic, based on negative results in bacterial mutation test and chromosomal aberration test *in vitro*.

The production volume is ca. 250 tonnes/year in 1996 in Japan. All of this produced in Japan is used as monomer unit of polyester, and no consumer use is reported.

A generic fugacity model (Mackey level III) shows that this chemical will distribute mainly into the water phase (87.9%) when it is discharged into water.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE

FULL SIDS SUMMARY

CAS NO: 840-65-3		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point			192.2 °C
2.2	Boiling Point			> 300 °C
2.3	Density			
2.4	Vapour Pressure		OECD TG104	3.3×10^{-4} Pa at 25 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	3.5
2.6 A.	Water Solubility		OECD TG 105	0.15 mg/L at 25 °C
B.	pH			
	pKa			
2.12	Oxidation: Reduction Potential			
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation			
3.1.2	Stability in Water		OECD TG 111	$T_{1/2}$ = Stable in pH 4 at 25 °C $T_{1/2}$ = 65.9 days at pH7 at 25 °C $T_{1/2}$ = 1.04 days at pH9 at 25 °C
3.2	Monitoring Data			None
3.3	Transport and Distribution		Calculated (Fugacity Level III type)	Release: 100% to Water In Air 0.7 % In Water 87.9 % In Sediment 4.4 % In Soil 7.1 %
			(local exposure)	1.1×10^{-5} mg/L (Japan)
3.5	Biodegradation		OECD 301C	7 % by HPLC after 28 days
3.7	Bioaccumulation		OECD 305C	BCF: 6.1 - 63
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	*Oryzias latipes*	OECD TG 203	LC_{50}(48hr): > 0.1 mg/l LC_{50}(96hr): > 0.1 mg/l LC_{50}(14 d): > 0.1 mg/l
4.2	Acute Toxicity to Aquatic Invertebrates *Daphnia*	*Daphnia magna*	OECD TG 202	EC_{50}(48hr): > 0.1 mg/l EC_{50}(48hr): > 0.1 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	*Selenastrum capricornutum*	OECD TG 201	EC_{50}(72hr): > 0.1 mg/l NOEC; > 0.1 mg/l
4.5.2	Chronic Toxicity to Aquatic Invertebrates (*Daphnia*)	*Daphnia magna*	OECD TG 202	EC_{50}(21d,Repro): > 0.02 mg/l NOEC: > 0.02 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

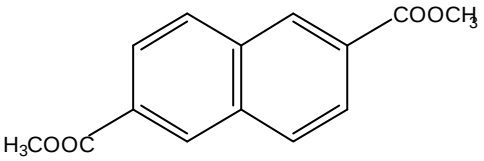
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	OECD TG 401	LD_{50} = >2,000 mg/kg b.w.
5.1.2	Acute Inhalation Toxicity			No data
5.1.3	Acute Dermal Toxicity			No data
5.4	Repeated Dose Toxicity	Rat	OECD Combined	NOAEL = 1,000 mg/kg/day
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	S. typhimurium E. coli WP2	Japanese TG and OECD TG 471 & 472	- (With metabolic activation) - (Without metabolic activation)
B.	Non-Bacterial In Vitro Test (Chromosomal aberrations)	Chinese hamster CHL cells	Japanese TG and OECD TG 473	- (With metabolic activation) - (Without metabolic activation)
5.6	Genetic Toxicity In Vivo			No data
5.8	Toxicity to Reproduction	Rat	OECD combined	NOAEL = 1,000 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity			No data
5.11	Experience with Human Exposure			No data

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

SIDS INITIAL ASSESSMENT REPORT

1. IDENTITY

- OECD Name: Dimethyl 2,6-naphthalenedicarboxylate
- Synonym: 2,6-Naphthalenedicarboxylic acid dimethyl ester
- CAS Number: 840-65-3
- Empirical Formula: $C_{14}H_{12}O_4$
- Structural Formula:



- Degree of Purity: 99.91
- Major Impurity: None
- Essential Additives: None
- Physical-chemical properties
  - Melting Point: 192.2 °C
  - Vapour pressure: 3.3×10^{-4} Pa at 25 °C
  - Water solubility: 0.15 mg/L
  - Log Pow: 3.5

2. GENERAL INFORMATION ON EXPOSURE

2.1 Production and import

The production volume of dimethyl 2,6-naphthalenedicarboxylate in Japan is 1,159 tonnes/year in 1995.

2.2 Use pattern

All of dimethyl 2,6-naphthalenedicarboxylate produced in Japan is used as monomer unit of polyester, and no consumer use is reported.

2.3 Other information

None

3. ENVIRONMENT

3.1 Environmental Exposure

3.1.1 General Discussion

Dimethyl 2,6-naphthalenedicarboxylate is not biodegradable (OECD 301C: Ca.7 % after 28d) and relatively stable in water under acidic condition. Although direct photodegradation is expected

because dimethyl 2,6-naphthalenedicarboxylate has absorption band in UV and VIS region, the data of half-lifetime is not available.

Dimethyl 2,6-naphthalenedicarboxylate is moderately bioaccumulative (BCF 6.1 – 63, Carp).

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

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

Compartment	Release 100% to air	Release 100% to water	Release 100% to soil
Air	11.6 %	0.7 %	0.0 %
Water	10.3 %	87.9 %	0.4 %
Soil	77.2 %	4.4 %	99.6 %
Sediment	0.8 %	7.1 %	0.0 %

As this chemical is used in closed system as a monomer unit of polyester and is not included in consumer products, its release to the environment may occur only from the production cite.

3.1.2 Predicted Environmental Concentration

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

a. Regional exposure

According to report from a Japanese manufacturer whose production volume is 250 t/y, 146 kg/year (measured) of dimethyl 2,6-naphthalenedicarboxylate are released with 1.35×10^{10} L/year of effluent into sea. Local Predicted Environmental Concentration (PEC_{local}) is calculated to be 1.1×10^{-5} mg/L as a worst case scenario, employing the following calculation model and dilution factor of 1000(default).

Amount of release (1.46×10^{8} mg/y)
Volume of effluent (1.35×10^{10} L/y) x Dilution Factor (1000)

3.2 Effects on the Environments

3.2.1 Effects on aquatic organisms

Acute and chronic toxicity data of dimethyl 2,6-naphthalenedicarboxylate to aquatic organisms are summarized below (Table 2). Toxicity of this chemical seems low because most toxicity data were

higher than > 0.1 mg/l, the maximum dispersible concentration by a dispersant (a mixture of tetrahydrofuran (THF) and HCO-30 (hydrogenated castor oil), 8 % and 92 % each) with final concentration of 100 mg/l (a limit by OECD test guideline). However, HCO-50 was used in the reproduction test of *D. magna*. Because some side effects of HCO-30 appeared in a preliminary reproduction test as decrease in number of offspring and appearance of unhealthy adults. As a result, the maximum dispersible concentration of test substance decreased to 0.02 mg/l by 30 mg/l of dispersant (1.6 mg/l TMF and 28.4 mg/l HCO-50, each) in the reproduction test of *D. magna*.

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. As the lowest toxicity data, 21-d NOEC of *Daphnia magna* (reproduction), > 0.02 mg/l, was adopted (Table 2). The assessment factor of 100 was used 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.

As a lowest data 21-d EC50 (> 0.02 mg/l) of *Daphnia magna* was selected.

Thus, PNEC of this chemical is calculated as below

PNEC = (> 0.02) / 100 = > 0.0002 mg/l

Table 2

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

Species	Endpoint	Conc. (mg/l)	Remarks
Selenastrum capricornutum (algae)	Bms 72 h EC50	> 0.1	a, 1), A
	Bms 72 h NOEC	> 0.1	c, 1), C
Daphnia magna (Water flea)	Imm 24 h EC50	> 0.1	a, 1), A
	Rep 21 d EC50	> 0.02	c, 1)
	Rep 21 d NOEC	> 0.02	c, 1), C
Oryzias latipes (fish, Medaka)	Mor 96 h LC50	> 0.1	a, 1)
	Mor 14-d LC50	> 0.1	a, 1), A

Notes: Bms; biomass, Mor; mortality, Rep; reproduction,
A), C); the lowest values among the acute or chronic toxicity data of algae, Cladocera (water flea) and fishes to determine PNEC of this chemical.
1) Toxicity data of the tests were conducted by the Environment Agency of Japan based on OECD Test Guidelines and GLP.

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 > 0.0002 mg/l.

PEC from Japanese local exposure scenario is 1.1×10^{-5} mg/l.

PEC_{local} / PNEC = 1.1×10^{-5}/ (> 0.0002) = < 0.055 < 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

Dimethyl 2,6-naphthalenedicarboxylate is produced in closed systems and used for polyester resin synthesis. The occupational exposures are expected through inhalation and dermal route is assumed negligible because this chemical is solid. As the atmospheric concentration in plant was not measured, the maximum exposure levels are estimated according to working schedules as follows. If a single worker (body weight; 70 kg, respiratory volume; 1.25 m^3/hr) is assigned to implement this operation without protection, the highest daily intake (EHE) is calculated as 0.04 mg/kg/day as the worst case. Practically, workers always wear protective gloves and respiratory protective equipment (mask) during the operation.

	Frequency Times/day	Duration hr	Working hr/day	Maximum Concentration mg/m^3	Maximum EHE mg/kg/day
Bag Filling	1	2	2	1	0.04

EHE: Estimated Human Exposure

4.1.2 Consumer exposure

As dimethyl 2,6-naphthalenedicarboxylate is used as a raw material for polyethylenenaphthalate resin, liquid crystal, engineering plastic, etc., consumer exposure is not expected in sponsor country.

4.1.3 Indirect exposure via the environment

As dimethyl 2,6-naphthalenedicarboxylate is persistent in water and moderately 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. 1.1×10^{-5} mg/l. The daily intake through drinking water is calculated as 3.67×10^{-7} mg/kg/day (2 l/day, 60 kg b.w.).

Using the maximum bioconcentration factor of 63 obtained by tests, the concentration of this chemical in fish can be calculated as follows:

PEC_{fish} = (1.10 x 10^{-5} mg/l) x 63 = 6.93 x 10^{-7} 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 1.04 x 10^{-6} mg/kg/day.

4.2 Effects on Human Health

a) Acute toxicity

Any lethality in both sexes of rats by oral administration was not observed at dose of 2,000 mg/kg. Any toxic signs did not appear. [MHW, Japan (1997)]

b) Irritation

There are no available data.

c) Sensitisation

There are no available data.

d) Repeated toxicity

[SIDS data] Oral toxicity of dimethyl 2,6-naphthalenedicarboxylate in rats was studied by an OECD combined repeat dose and reproductive/developmental toxicity screening test. The chemical was administered by gavage at doses of 0, 30, 100, 300 and 1,000 mg/kg/day for 45 days in males and from 14 days before mating to day 3 of lactation in females. No effects of the test substance on males or females were noted. The NOAEL for repeat dose toxicity is considered to be 1,000 mg/kg/day for both sexes. [MHW, Japan (1997)]

e) Reproductive/developmental toxicity

[SIDS data] Oral toxicity of dimethyl 2,6-naphthalenedicarboxylate in rats was studied by an OECD combined repeat dose and reproductive/developmental toxicity screening test. The chemical was administered by gavage at doses of 0, 30, 100, 300 and 1,000 mg/kg/day for 45 days in males and from 14 days before mating to day 3 of lactation in females. No effects of the test substance on copulation, fertility, delivery or lactation were noted. The NOAEL for reproductive performance of males and females, and for pup development is considered to be 1,000 mg/kg/day. [MHW, Japan (1997)]

f) Genetic toxicity

Bacterial test

[SIDS data] Dimethyl 2,6-naphthalenedicarboxylate was not mutagenic in *Salmonella typhimurium* TA100, TA1535, TA98, TA1537 and *Escherichia coli* WP2 *uvr*A, with or without an exogenous metabolic activation system. [MHW, Japan (1997)]

Non-bacterial test *in vitro*

[SIDS data] Genotoxicity of dimethyl 2,6-naphthalenedicarboxylate was studied by chromosomal aberration test in cultured Chinese hamster lung (CHL/IU) cells. Structural chromosomal aberrations were not induced up to a maximum concentration of 2.4 mg/ml (10 mM) with continuous treatment, or by short-term treatment with and without an exogenous metabolic

activation system. Polyploidy was induced by continuous treatment with 2.4 mg/ml for 48 h. However, it was considered that dimethyl 2,6-naphthalenedicarboxylate did not induce chromosomal aberrations or polyploidy since the frequency was very low. [MHW, Japan (1997)]

4.3 Initial Assessment for Human Health

Oral LD_{50} of dimethyl 2,6-naphthalenedicarboxylate for rats is more than 2,000 mg/kg. There are no available data for irritation and sensitisation. In a combined repeat dose and reproductive/ developmental toxicity study, any toxic effects were not observed. Therefore, NOAEL was considered to be 1000 mg/kg/day for both repeated dose toxicity and reproductive toxicity. This chemical may not be genotoxic, based on negative results in bacterial mutation test and chromosomal aberration test in vitro.

Occupational exposure
Dimethyl 2,6-naphthalenedicarboxylate is produced and used in a closed system at industries and workers wear protective gloves and respiratory protective equipment during bag filling operation. As the route of occupational exposure 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 0.04 mg/kg/day as the worst case. Occupational risk is presumably low because the margin of safety is 2.50×10^{4}.

Consumer exposure
No consumer exposure is expected because this chemical is not used in consumer products.

Indirect exposure via environment
As for indirect exposure via environment, PEC_{local} of 1.10×10^{-5} mg/l from local exposure scenario was used for the estimation. The daily intakes through drinking water and fish are calculated as 3.67×10^{-7} mg/kg/day and 1.04×10^{-6} mg/kg/day, respectively. Since the margin of safety is very large, such as 2.73×10^{9} for drinking water and 9.62×10^{8} for fish, health risk via environment is presumably low.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Dimethyl 2,6-naphthalenedicarboxylate is not biodegradable (OECD 301C: ca. 7% after 28-d) and has relatively stable in water, and moderately bioaccumulative (BCF 6.1~ 63, Carp). Toxicity values to the test organisms were higher than the maximum dispersible concentrations, > 0.1 mg/l except for > 0.02 mg/l in the reproduction test of *Daphnia magna* conducted using a different dispersant. PEC/PNEC ratio (1.1×10^{-4}/(> 0.0002) = < 0.55) is less than 1 based on the local exposure scenario in the Sponsor country and NOEC in reproduction test of *D. magna*. It is currently considered of low potential risk to environments and low priority for further work.

Dimethyl 2,6-naphthalenedicarboxylate is not toxic in a repeated dose and reproductive toxicity studies, and not genotoxic. There is no information on irritation, sensitization and no consumer exposure. The margin of safety is more than 1×10^{4} via an occupational and indirect exposure. Therefore, it is currently considered of low potential human risk and low priority for further work.

5.2 Recommendations

No recommendation

6. REFERENCES

Ministry of Health and Welfare, Japan: *Toxicity Testing Reports of Environmental Chemicals* 5, 499-524 (1997).

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-Sendnersymbol 146 \f "Times New Roman" \s 11'}s equation (4). This equation is one of analytic solution led under the following conditions from diffusion equation.

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

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

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)
: 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 symbol 146 \f "Times New Roman" \s 11'}s equation (4) is simplified to equation (5)

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

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

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

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

P = 1 cm/sec (860 m/day)
= 3.14
d = 10 m
x = 1000 m

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

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

REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE 5 CHEMICAL

Dimethyl 2,6-naphthalenedicarboxylate

CAS No. 840-65-3

Sponsor Country: Japan

DATE: March 15, 1999

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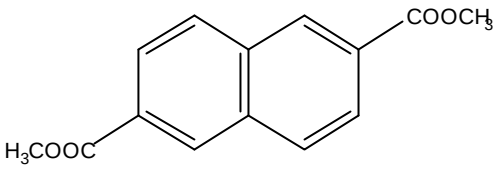
6. References

Appendix-1

Note: *; Data Elements In The Sids
†; Data Elements Specially Required For Inorganic Chemicals

S I D S P R O F I L E

1.01 A.	**CAS No.**	840-65-3
1.01 C.	**CHEMICAL NAME (OECD Name)**	Dimethyl 2,6-naphthalenedicarboxylate
1.01 D.	**CAS DESCRIPTOR**	
1.01 G.	**STRUCTURAL FORMULA**	
	OTHER CHEMICAL IDENTITY INFORMATION	
1.5	**QUANTITY**	1,159 tonnes/year in Japan
1.7	**USE PATTERN**	Intermediate in closed system
1.9	**SOURCES AND LEVELS OF EXPOSURE**	146 kg/year Release into bay
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)	SIDS testing required: Water solubility, Vapour pressure, Octanol/water partition coefficient Stability in water, Biodegradation Acute toxicity, Combined repeat dose and reproductive toxicity Gene mutation, Chromosomal aberration test in vitro	

S I D S S U M M A R Y

CAS NO: 840-65-3		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	N						N
2.4	Vapour Pressure	N						Y
2.5	Partition Coefficient	N						Y
2.6	Water Solubility	N						Y
	pH and pKa values	N						N
2.12	Oxidation: Reduction potential	N						N
	OTHER P/C STUDIES RECEIVED							
ENVIRONMENTAL FATE and PATHWAY								
3.1.1	Photodegradation	N						N
3.1.2	Stability in water	N						Y
3.2	Monitoring data	N						N
3.3	Transport and Distribution	N						N
3.5	Biodegradation	N						Y
	OTHER ENV FATE STUDIES RECEIVED							
ECOTOXICITY								
4.1	Acute toxicity to Fish	N						Y
4.2	Acute toxicity to Daphnia	N						Y
4.3	Toxicity to Algae	N						Y
4.5.2	Chronic toxicity to Daphnia	N						Y
4.6.1	Toxicity to Soil dwelling organisms	N						N
4.6.2	Toxicity to Terrestrial plants	N						N
4.6.3	Toxicity to Birds	N						N
	OTHER ECOTOXICITY STUDIES RECEIVED							
TOXICITY								
5.1.1	Acute Oral	N						Y
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** 840-65-3

B. Name *(IUPAC name)* Dimethyl 2,6-naphthalenedicarboxylate

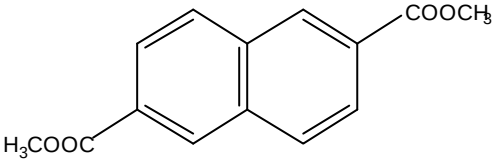
***C. Name** *(OECD name)* Dimethyl 2,6-naphthalenedicarboxylate

†D. CAS Descriptor

E. EINECS-Number 212-661-4

F. Molecular Formula $C_{14}H_{12}O_4$

***G. Structural Formula**



H. Substance Group

I. Substance Remark

J. Molecular Weight 244.25

1.02 OECD INFORMATION

A. Sponsor Country: Japan

B. Lead Organisation:

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

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

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

C. Purity 99.91 %

1.2 SYNONYMS 2,6-Naphthalenedicarboxylic acid dimethyl ester

1.3 IMPURITIES

None

1.4 ADDITIVES

None

***1.5 QUANTITY**

Remarks: 1,159 tonnes/year
Reference: MITI, Japan

1.6 LABELLING AND CLASSIFICATION

None

***1.7 USE PATTERN**

A. General

Type of Use:	**Category:**
main	Intermediate
industrial	Intermediate in closed system
use	Intermediate

Remarks: None
Reference: MITI, Japan

1.8 OCCUPATIONAL EXPOSURE LIMIT

None

*** 1.9 SOURCES OF EXPOSURE**

In Japan, this chemical is produced in 1 company.

Source:	Media of release: Bay Quantities per media: 146 kg/year
Remarks:	
Reference:	MITI, Japan

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT**

Value:	192 °C
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Sublimation:	Yes **[ ]** No **[ ]** Ambiguous **[ ]**
Method:	
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	
Reference:	Company data

***2.2 BOILING POINT**

Value:	> 300 °C
Pressure:	1,018 Pa
Decomposition:	Yes **[ ]** No **[X]** Ambiguous **[ ]**
Method:	
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Remarks:	
Reference:	MITI, Japan

***2.4 VAPOUR PRESSURE**

Value:	3.3×10^{-4} Pa
Temperature:	25 °C
Method:	calculated **[ ]**; measured **[X]** OECD TG 104
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	
Reference:	MITI, Japan.

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

Log Pow:	3.5
Temperature:	25 °C

Method:	calculated **[ ]**; measured **[** X **]** OECD TG 107 HPLC method
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	
Reference:	MITI, Japan

***2.6 WATER SOLUBILITY**

A. Solubility

Value:	0.15 mg/l
Temperature:	25 °C
Description:	Miscible **[ ]**; Of very high solubility **[ ]**; Soluble **[ ]**; Slightly soluble **[ ]**; Of low solubility **[ ]**; Of very low solubility **[X]**; Not soluble **[ ]**
Method:	OECD TG 105
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	
Reference:	MITI, Japan

B. pH Value, pKa Value

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

***3.1.2 STABILITY IN WATER**

Type:	Abiotic (hydrolysis) **[X]**; biotic (sediment)**[ ]**
Half life:	Stable in pH 4 at 25 °C 65.9 days in pH 7 at 25 °C 1.04 days in pH 9 at °C
Method:	OECD TG 111
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	
Reference:	MITI, Japan

***3.2 MONITORING DATA (ENVIRONMENTAL)**

No studies located

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	11.6 %	0.7 %	0.0 %
Water	10.3 %	87.9 %	0.4 %
Soil	77.2 %	4.4 %	99.6 %
Sediment	0.8 %	7.1 %	0.0 %

Remarks: Appendix 1

Reference: MITI. Japan

*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: 6 % by BOD after 28 days
7 % by HPLC 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: purity: 99.9 %

Remarks: partially degraded to carboxylic acid and methanol

Reference: MITI, Japan

3.7 BIOACCUMULATION

Species: Carp (*Cyprinus carpio*)

Exposure period: 6 weeks

Temperature: 25 °C

Concentration: (1) 0.1 mg/L
(2) 0.01 mg/L

BCF: (1) 6.1 – 63
(2) 7.1 – 23

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: purity: 99.9 %

Remarks:

Reference: MITI, Japan

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

(a)

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:	LC_{50} (96h) > 0.1 mg/l
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD TG 203 (1992)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.91 %
Remarks:	Group of 10 Himedaka were exposed to measured concentration of 0.1 mg/l*, solubilizer (tetrahydrofuran (THF) 8.0 mg/l, hydrogenated castor oil (HCO-30) 92.0 mg/l) control and laboratory water control (dechlorinated tapwater). The LC_{50} (96h). * 0.1 mg/l is the highest concentration that DND could be dispersed.
Reference:	Environment Agency of Japan (1996)

(b)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other *(e.g. field test)* **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Oryzias latipes* (Himedaka)
Exposure period:	14 d
Results:	LC_{50} (14d) > 0.1 mg/l
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD TG 203 (1992)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.91 %
Remarks:	Group of 10 Himedaka were exposed to measured concentration of 0.1 mg/l*, solubilizer (THF 8.0 mg/l, HCO-30 92.0 mg/l) control and laboratory water control. * 0.1 mg/l is the highest concentration that DND could be dispersed.
Reference:	Environment Agency of Japan (1996)

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:	48 h

Results:	EC_{50} (48h) > 0.1 mg/l
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD TG 202
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.91 %
Remarks:	20 daphnids (4 replicates; 5 organisms per replicate) were exposed to measured concentration of 0.1 mg/l*, solubilizer (THF 8.0 mg/l, HCO-30 92.0 mg/l) control and laboratory water control. * 0.1 mg/l is the highest concentration that DND could be dispersed.
Reference:	Environment Agency of Japan (1996).

*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 EC_{50} (72h) > 0.1 mg/l *(Endpoint)* NOEC > 0.1 mg/l
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD TG 201 (1984) open-system **[ ]**; closed-system **[X]**
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.91 %
Remarks:	Static test. The EC_{50} value for biomass was calculated based on measured concentration (0.1 mg/l*). THF (4.0 mg/l) and HCO-30 (96.0 mg/l) was used as solubilizer. * 0.1 mg/l is the highest concentration that DND could be dispersed.
Reference:	Environment Agency of Japan (1996)

4.4 TOXICITY TO BACTERIA

No data

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

No data

4.5.1 CHRONIC TOXICITY TO FISH

(*) 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:EC_{50} (21 d) > 0.02 mg/l *(Endpoint)* NOEC > 0.02 mg/l
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD TG 202 (1984)
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	As prescribed by 1.1 - 1.4, purity: 99.91 %
Remarks:	Forty daphnids (4 replicates; 10 daphnids per replicate) were exposed to nominal concentration of 0.02* mg/l (measured concentration; 0.018 mg/l at the start of exposure, 0.007 and < 0.001 mg/l after 1 and 2 days, respectively), solubilizer control (THF, 1.6 mg/l and HCO-50, 28.4 mg/l) or laboratory water control (dechlorinated tap water). The test water was renewaled with 2 or 3 d cycles. * 0.02 mg/l is the highest concentration that DND could be dispersed.
Reference:	Environment Agency of Japan (1996)

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

No data

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

No data

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

No data

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

No data

4.8 BIOTRANSFORMATION AND KINETICS

No data

4.9 ADDITIONAL REMARKS

None

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	Rat/Cij; CD (SD)
Value:	>2,000 mg/kg b.w. for male and female
	Discriminating dose: 0, 500, 1,000 and 2,000 mg/kg
Method:	OECD TG 401
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	No toxicity
Reference:	MHW, Japan: 1997

5.1.2 ACUTE INHALATION TOXICITY

No available data

5.1.3 ACUTE DERMAL TOXICITY

No available data

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

No available data

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

No available data

5.2.2 EYE IRRITATION/CORROSION

No available data

5.3 SKIN SENSITISATION

No available data

*5.4 REPEATED DOSE TOXICITY (SIDS data)

Species/strain:	Rats/Crj; CD (SD)
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Route of Administration:	Oral (by gavage)
Exposure period:	Males; 49 days,
	Females; from 14 days before mating to day 3 of lactation
Frequency of treatment:	Daily
Post exposure observation period:	
Dose:	30, 100, 300, 1,000 mg/kg/day (in 0.5 % Na-CMC)
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**;
	Concurrent no treatment**[ ]**; Concurrent vehicle **[X]**;Historical**[ ]**
NOAEL:	Male: 1,000 mg/kg/day
	Female: 1,000 mg/kg/day

Results: Any toxicological effects were not observed.
Method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: purity: 99.9 %
Reference: MHW, Japan: 1997

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: Bacterial reverse mutation assay
System of testing: *Salmonella typhimurium* TA100, TA1535, TA98, TA1537
Escherichia coli WP2 *uvr*A
Concentration: -S9: 0, 313, 625, 1250, 2500, 5000 µg /plate
+S9: 0, 313, 625, 1250, 2500, 5000 µg /plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone.
Results:
Cytotoxicity conc: Toxicity was not observed at 5000 µg/plate in five strains with or without an S9 mix.
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: purity: 99.9 %
Remarks:
Reference: MHW, Japan: 1997

NON-BACTERIAL IN VITRO TEST

Type: Chromosomal aberration test
System of testing: CHL/IU cell
Concentration: -S9 (continuous treatment): 0, 0.60, 1.2, 2.4 mg/ml
-S9 (short-term treatment): 0, 0.60, 1.2, 2.4 mg/ml
+S9 (short-term treatment): 0, 0.60, 1.2, 2.4 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:
Precipitation conc:
Genotoxic effects:

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

Method:	Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD TG (473).
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	Structural chromosomal aberrations were not induced in any treatment group. With continuous treatment for 48 h, polyploidy (1.25 %) was weakly induced at 2.4 mg/ml (high concentration).
Reference:	MHW, Japan: 1997

* 5.6 GENETIC TOXICITY IN VIVO

No available data

5.7 CARCINOGENICITY

No available 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 (gavage)
Exposure period:	Male: For 2 weeks prior to mating and 2 weeks of mating Female: For 2 weeks prior to mating, 2 weeks of mating and throughout pregnancy until day 3 postpartum
Frequency of treatment:	Daily
Post exposure observation period:	
Premating exposure period:	male: 14 days, female: 14 days
Duration of the test:	
Dose:	30, 100, 300, 1,000 mg/kg/day (in 0.5 % Na-CMC)
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment**[ ]**;Concurrent vehicle **[X]**; Historical **[ ]**
NOAEL Parental:	Male; 1,000 mg/kg, Female; 1,000 mg/kg
NOAEL F1 Offspring:	1,000 mg/kg
Results:	Any toxicity was not observed.
Method:	OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	purity: 99.9 %
Remarks:	
Reference:	MHW, Japan: 1997

*5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

No available data

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

No available data

B. Toxicodynamics, toxicokinetics

No available data

*** 5.11 EXPERIENCE WITH HUMAN EXPOSURE**

No available data

6. REFERENCES

Ministry of Health and Welfare, Japan: *Toxicity Testing Reports of Environmental Chemicals* 5, 499-524 (1997).

Appendix 1

scenario 1

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	1,000	7.1.E-06	7.1.E+04	11.6	1.8E+02	7.1.E+02
water	0	3.2.E-03	6.3.E+04	10.3	5.1E+00	6.3.E+01
soil	0	3.0.E-01	4.7.E+05	77.2	3.8E+01	
sediment		5.1.E-02	5.1.E+03	0.8	4.1E-01	1.0.E-01
		total amount	6.1.E+06			

scenario 2

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	0	6.3.E-07	6.3.E+03	0.7	1.6.E+01	6.3.E+01
water	1000	4.2.E-02	8.4.E+05	87.9	6.8.E+01	8.4.E+02
soil	0	2.6.E-02	4.2.E+04	4.4	3.4.E+00	
sediment		6.8.E-01	6.8.E+04	7.1	5.4.E+00	1.4.E+00
		total amount	9.6.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-07	1.2.E+03	0.0	3.2.E+00	1.2.E+01
water	0	2.1.E-03	4.1.E+04	0.4	3.3.E+00	4.1.E+01
soil	1000	7.3.E+00	1.2.E-07	99.6	9.4.E+02	
sediment		3.3.E-02	3.3.E+03	0.0	2.7.E-01	6.6.E-02
		total amount	1.2.E+07			

scenario 4

	emission rate	conc.	amount	percent	transformation rate [kg/h]	
	[kg/h]	[g/m^3]	[kg]	[%]	reaction	advection
air	600	4.5.E-06	4.5.E+04	2.4	1.1.E+02	4.5.E+02
water	300	1.5.E-02	3.0.E+05	16.1	2.4.E+01	3.0.E+02
soil	100	9.2.E-01	1.5.E+06	80.2	1.2.E+02	
sediment		2.4.E-01	2.4.E+04	1.3	1.9.E-00	4.7.E-01
		total amount	1.8.E+06			

Physico-chemical parameter

molecular weight		244.25	Measured
melting point		199.2	Measured
vapor pressure [Pa]		3.30E-04	Measured
water solubility [g/m^3]		0.15	Measured
log Kow		3.5	Measured
half life [h]	in air	272	Estimated
	in water	8640	Estimated
	in soil	8640	Estimated
	in sediment	8640	Estimated

Temp. []	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