

Safety Summary Sheet

Terephthalic acid (CAS NO. 100-21-0)

Terephthalic acid (CAS NO.: 100-21-0)		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		Unknown	>300, 402, 425°C
2.2	Boiling Point		Unknown	Sublime
2.3	Density		DIN 5314 Not specified Not specified	Bulk density : 1.12 g/cm ³ Density : 1.5 g/cm ³ Density : 1.51 g/cm ³
2.4	Vapour Pressure		Not specified	3 × 10 ⁻¹⁰ hPa (20 °C) (extrapolated from vapor pressures measured at temperatures between 250 and 427 °C)
2.5	Partition Coefficient (log Kow)		Not specified	LogKow : 2
2.6.1A	Water Solubility		Not specified Not specified	15 mg/l (10 °C) (not soluble) 19 mg/l (25 °C) (not soluble)
2.6.1.B	Dissociation Constant (pKa)		Not specified	pKa1 : 3.52, pKa2 : 4.46 (25 °C)
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		Calculation by AopWin v1.90	half life : 8.647 days reaction rate constant with hydroxyl radicals: 1.2370x10 ⁻¹² cm ³ /mol-sec
3.1.2	Stability in Water			No data
3.1.3	Stability in Soil			No data
3.2	Monitoring Data		Surface water, bottom sediment Atmospheric concentration ; air Sewage plant drainage; surface water	Surface water : 0.060-0.12 μ g/l (detected from 2 out of 23 areas in Japan, 2002) Bottom sediment : 10-20 ng/g dry weight (detected from 4 out of 21 areas in Japan, 2002) 11.1 ng/m ³ (average of 6 days; max. 23 ng/m ³) (Japan, 1990 [reported]) 13 ng/l (Washington D.C., US, 1975) 5.3 μ g/l (Japan, 1975)
3.3.1	Transport between Environmental Compartments		Calculation by Fugacity Level III model (EPIWIN v. 3.05, MW 166.13, LogKow 2.00, vapour pressure 1.19x10 ⁻⁵ mmHg 25 °C , water solubility 15mg/l 20°C)	Air : 0.000012% Water : 32.7% Soil : 67.2% Sediment : 0.098%
3.3.2	Distribution (Koc etc.)		Calculation by PCKOCWIN v.1.66	LogKoc : 1.855

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3.4	Biodegradation		OECD TG 301 C (Ready Biodegradability: Modified MITI Test (I)) OECD TG 301 B (Ready Biodegradability: Modified Sturm Test) etc.	74.7% (O ₂ consumption, 14 d) 99.3% (UV-VIS, 14 d) 100% (HPLC, 14 d) Readily biodegradable (supported by a lot of test reports)
3.5	BOD-5, COD or BOD-5/ COD ratio			No data
3.6	Bioaccumulation		Calculation by EPIWIN (unspecified version)	BCF: 2
ECOTOXICOLOGY				
4.1	Acute Toxicity to Fish	<i>Oryzias latipes</i> <i>Leuciscus idus melanotus</i> <i>Salmo gairdneri</i> <i>Brachydanio rerio</i>	OECD TG 203 (Fish, Acute Toxicity Test) OECD TG 203 (Fish, Acute Toxicity Test, static) OECD TG 203 (Fish, Acute Toxicity Test, semi-static) OECD TG 203 (Fish, Acute Toxicity Test, static)	LC ₅₀ (96h) : >19 mg/l LC ₅₀ (96h) : >1000 mg/l* NOEC (96h) : >=1000 mg/l* LC ₅₀ (96h) : 798-1640 mg/l (mean value 1157 mg/l)* LC ₀ (96h) : >500 mg/l*
4.2	Acute Toxicity to Aquatic Invertebrates (Daphnia etc.)	<i>Daphnia magna</i> <i>Daphnia magna</i>	OECD TG 202 (Daphnia sp. Acute Immobilisation Test) OECD TG 202 (Daphnia sp. Acute Immobilisation Test, static)	EC ₅₀ (48h) : >20 mg/l* EC ₅₀ (48h) : >1000 mg/l* NOEC (48h) : 600 mg/l*
4.3	Toxicity to Aquatic Plants (Algae etc.)	<i>Selenastrum capricornutum</i> (new name: <i>Pseudokirchnerella subcapitata</i>) <i>Selenastrum capricornutum</i> (new name: <i>Pseudokirchnerella subcapitata</i>)	OECD TG 201 (Alga, Growth Inhibition Test) OECD TG 201 (Alga, Growth Inhibition Test, static)	Growth rate : EC ₅₀ (72h) : >18 mg/l NOEC (72h) : 18 mg/l Biomass: EC ₅₀ (72h) : >19 mg/l NOEC (72h) : 19 mg/l Biomass: EC ₅₀ (96h) : >1000 mg/l * NOEC (96h) : >1000 mg/l*

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4.4	Toxicity to Microorganisms (Activated Sludge Respiration Inhibition test etc.)	Activated sludge (predominantly domestic sewage) <i>Fasciola hepatica</i> (protozoa) <i>Tetrahymena pyriformis</i> (protozoa) <i>Caenorhabditis elegans</i> (nematode)	OECD TG 209 (Activated sludge, Respiration Inhibition Test, static) Unknown Unknown (motility inhibition) Unknown	EC ₅₀ (16d) : 1392.8 mg/l* EC ₀ (2h) : 830 mg/l* EC ₅₀ (24h) : 800 mg/l* EC ₀ (unknown period) : 1 μg/l
4.5.1	Chronic Toxicity to Fish			No data
4.5.2	Chronic Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD TG 211 (Daphnia magna Reproduction Test)	EC ₅₀ (21d) : >20 mg/l NOEC (21d) : 20 mg/l
4.6	Toxicity to Terrestrial Organisms	<i>Avena sativa</i> <i>Oryza sativa</i> <i>Drosophila melanogaster</i>	Unknown Unknown Unknown	EC ₀ (seedling root elongation; 1d) : 100 mg/l* EC ₀ (seedling root elongation; 5d) : >10 mg/l EC ₂₀ (seedling root elongation; 5d) : 100 mg/l* LC ₀ (mortality, 3d): 166 mg/kg bw
4.6.1	Toxicity to Sediment Dwelling Organisms			No data
TOXICOLOGY				
5.1	Toxicokinetics, Metabolism and Distribution	Rat Rat	Unknown Unknown (Feto-placental Transfer)	absorbed rapidly, distributed mainly to kidney and excreted to urine as terephthalic acid, Transported to the fetus, however the concs. in fetus tissues were low relative to the corresponding maternal ones.
5.2	Acute Toxicity			
A.	Acute Oral Toxicity	Rat	Unknown	LD50 : >5000 mg/kg
B.	Acute Inhalation Toxicity	Rat	Unknown	LC50 : >2.02 mg/L (2hr)
C.	Acute Dermal Toxicity	Rabbit	Unknown	LD50 : >2000 mg/kg
D.	Acute Toxicity, Other Routes			No data
5.3	Irritation/Corrosion			
A.	Skin Irritation/Corrosion			No data
B.	Eye Irritation/Corrosion			No data
5.4	Skin Sensitization			No data

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5.5	Repeated Dose Toxicity	Rat	Unknown (oral feed, 15 wks)	NOAEL : male ; 1220 mg/kg/day female ; 1456 mg/kg/day
		Rat	Unknown (oral feed, 2 yrs)	NOAEL : male ; 142 mg/kg/day female ; <20 mg/kg/day
		Rat	Unknown (inhalation, 14 wks)	NOAEL : 1.2 mg/m ³
5.6	Genetic Toxicity in vitro			
A.	Gene Mutation (Bacterial Test etc.)	<i>S. typhimurium</i> and <i>E. coli</i>	Method by Japanese Industrial Safety and Health Act	Negative
B.	Chromosomal Aberration	CHL/IU	Unknown	Negative
5.7	Genetic Toxicity in vivo	Mouse	OECD TG 474 (Micronucleus assay, ip)	Negative
5.8	Carcinogenicity	Rat	Unknown (oral feed, 2 yrs)	male ; no tumors female ; bladder tumors at 1000mg/kg/day, which is believed to be caused by bladder calculi and unlikely for human (OECD SIAR)
5.9	Toxicity to Reproduction			
A.	Toxicity to Fertility	Rat	Unknown (oral feed, one-generation study)	NOAEL : Reproductive. ; 2480~3018mg/kg/day Parental & pups ; 240~307mg/kg/day
B.	Developmental Toxicity/Teratogenicity	Rat	Unknown (inhalation)	NOAEL : Maternal & developmental ; 10.0 mg/L Not teratogenic
5.10	Other relevant information			No data
5.11	Experience with Human Exposure			No data

* : greater than the solubility in water

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