

Safety Summary Sheet

1,3-Diphenylguanidine (CAS NO. 102-06-7)

1,3-Diphenylguanidine (CAS NO.: 102-06-7)		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		Differential scanning calorimetry	147~150°C
2.2	Boiling Point		Differential scanning calorimetry	>200°C (1.013×10 ⁵ Pa)
2.3	Density		Unknown	1.13 g/cm ³ (at 20°C)
2.4	Vapour Pressure		Extrapolation from measured data at 87-128°C	1.74×10 ⁻⁶ Pa (at 20°C)
2.5	Partition Coefficient (log Kow)		Calculated data	2.9
2.6.1A	Water Solubility		Similar to OECD TG 105	475 mg/L (at 20°C, pH7)
2.6.1.B	Dissociation Constant (pKa)		Unknown	10.12
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		Aqueous solution (incl. 1% acetonitrile) exposed to sunlight for 7days Calculation by AopWin v1.92	No photolysis observed in water Photodegradation in air : T1/2 : 0.125day
3.1.2	Stability in Water		At 80 °C , pH3.5, 7.0 and 10	pH3.5 : no hydrolysis after 500hrs pH7.0 : hydrolysis of 18.1% after 1000hrs pH10 : T1/2 ; 168hrs
3.1.3	Stability in Soil			No data
3.2	Monitoring Data		Detail unknown (MOE of Japan monitoring data, 1978)	<LOD both in surface water and in sediment (42 samples) (LOD : 2-5µg/L for surface water, 0.1-0.5mg/kg for sediment)
3.3.1	Transport between Environmental Compartments		Calculation by Fugacity Level III model (EPI WIN ver.3.12)	Air : 5.67×10 ⁻⁵ % Water : 13.3% Soil : 86.5% Sediment : 0.238%
3.3.2	Distribution (Koc etc.)			No data
3.4	Biodegradation	Adapted activated sludge	Similar to OECD TG 301D Closed	ca. 75% degraded after 28day (inherently biodegradable)

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			bottle method	
3.5	BOD-5, COD or BOD-5/ COD ratio		Unknown	BOD-5 : 2.3% (referred to TOD)
3.6	Bioaccumulation	Carp	OECD TG 305C	BCF <20
ECOTOXICOLOGY				
4.1	Acute Toxicity to Fish	Fathead minnow	Static (US EPA Ecological Research series 660/3-75009)	96hr LC50 : 4.2mg/L
4.2	Acute Toxicity to Aquatic Invertebrates (Daphnia etc.)	<i>Daphnia magna</i>	Static (US EPA Ecological Research series 660/3-75009)	48hr EC50 : 17 mg/L
4.3	Toxicity to Aquatic Plants (Algae etc.)	<i>Selenastrum capricornutum</i>	Static (US EPA , 1971, Algae assay procedure: bottle test)	96hr EC50 : 1.7 mg/L 96hr NOEC : 0.3 mg/L
4.4	Toxicity to Microorganisms (Activated Sludge Respiration Inhibition test etc.)	Activated sludge	OECD TG 209 Activated sludge, respiration inhibition test	3hr EC50 : 147 mg/L
4.5.1	Chronic Toxicity to Fish			No data
4.5.2	Chronic Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD TG 202 (Part2)	21day NOEC : 0.6 mg/L
4.6	Toxicity to Terrestrial Organisms	<i>Brassica rapa</i> Soil microorganisms Red winged blackbirds, Starlings and Passer domesticus	BBA Guideline 1984 (endpoint : growth) Unknown (endpoint : mortality) Single oral application (endpoint : mortality)	16day EC50 : 358 mg/kg soil dw, 16day NOEC : 100 mg/kg soil dw 4day LC50 : <0.1% LC50 : >100 mg/kg
4.6.1	Toxicity to Sediment Dwelling Organisms			No data
TOXICOLOGY				

1,3-Diphenylguanidine (CAS NO.: 102-06-7)		SPECIES	PROTOCOL	RESULTS
5.1	Toxicokinetics, Metabolism and Distribution	Rat	Unknown	Immediately absorbed and distributed after oral administration Within 24hr, 80% of dosing is excreted in urine and feces
5.2	Acute Toxicity			
A.	Acute Oral Toxicity	Rat	OECD TG 401	LD50 : male ; 111 mg/kg female ; 107 mg/kg
B.	Acute Inhalation Toxicity			No data
C.	Acute Dermal Toxicity	Rabbit	EEC N°L251/103 part B3	LD0 : >2000 mg/kg
D.	Acute Toxicity, Other Routes			No data
5.3	Irritation/Corrosion			
A.	Skin Irritation/Corrosion	Rabbit	Similar to OECD TG 404	Not irritating*1
B.	Eye Irritation/Corrosion	Rabbit	Similar to OECD TG 405	Corrosive*1
5.4	Skin Sensitization	Guinea pig	OECD TG 406 (GPMT)	Not sensitizing
5.5	Repeated Dose Toxicity	Rat	OECD TG 408 (90 day, oral feed)	NOAEL : 500 ppm (32 mg/kg/day)
5.6	Genetic Toxicity in vitro			
A.	Gene Mutation (Bacterial Test etc.)	<i>S. typhimurium</i> and <i>E. coli</i>	OECD TG 471	Negative
B.	Chromosomal Aberration	CHL/IU	OECD TG 473	Negative
5.7	Genetic Toxicity in vivo	Rat	OECD TG 475 Chromosomal Aberration assay (oral gavage)	Negative
		Mouse	Micronucleus assay (method by McGregor et al., oral feed)	Male ; Negative Female ; Equivocal
5.8	Carcinogenicity			No data
5.9	Toxicity to Reproduction			
A.	Toxicity to Fertility			No data*2
B.	Developmental Toxicity/Teratogenicity	Rat	EPA Health Effects Guidelines 560/6-82-001 (oral gavage)	NOAEL : Maternal ; 5 mg/kg/day Fetal ; 25 mg/kg/day Not teratogenic
5.10	Other relevant information			No data
5.11	Experience with Human Exposure	Human	Patch test	sensitizing

*1 : unpublished in-house data

*2 : 1,3-Diphenylguanidine did not affect the fertility of male mice when administered by gavage up to the maximal tested dose level of 16 mg/kg/d.

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