201-15110B

For CAS No. 2440-22-4:

WATER SOLUBILITY

Test substance:	2(2'- Hydroxy-5'-(methylphenyl) benzotriazole CAS No. 2440-22-4 Batch No. 07765CN2
Method:	The study was conducted under OECD Guideline No. 105. A 1.00 mg a.i/mL of Tinuvin P primary stock solution was prepared by placing 0.1003 g of the test substance in a 100-mL volumetric flask and bringing to volume with methanol. Three stock solutions were used to prepare calibration standards. A preliminary test was carried out to estimate the solubility. A definitive test was carried out with three aliquots, 0.5020, 0.5017, and 0.5014 g, of the test substance in a 250 mL round bottom flasks. To each flask, 100 mlL of distilled water was added and the flasks were agitated, one for 24 hours, a second flask for 48 hours, and the third for 72 hours. The temperature was measured and recorded daily during testing. The pH was measured at the conclusion of the 24-hour incubation period.[1]
Temperature:	20 °C
GLP:	Yes
Year:	2004
Results:	The mean water solubility and standard deviation for Tinuvin P was determined to be 0.173 ± 0.0206 mg/L at 20° C using shake-flask method.
Remarks:	This study was assigned a reliability code of 1a (GLP guideline study) according the criteria established by Klimisch *et al* (1997).[2]
References:	[1] Tinuvin P – Determination of Water Solubility. Study No. 13658.6246, Springborn Smithers Laboratories, 12 January 2004.

[2] Klimisch, H.J., Andreae, M and Tillman, U. A systemic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regulatory Toxicology and Pharmacology*. 25:1-5, 1997.

ACUTE TOXICITY TO FISH

Test substance:	2(2'- Hydroxy-5'-(methylphenyl) benzotriazole CAS No. 2440-22-4 Batch No. 07765CN2
Method:	This study was conducted under OECD Guideline No. 203 (Paris, 1984) under static-renewal test conditions. The toxicity test was conducted in 20.8 L glass aquaria, each containing 15 L of test solution. Test vessels were placed in a temperature-controlled waterbath designed to maintain test solution temperatures at 14 ± 1°C. The test area was illuminated with fluorescent lights at an intensity of 54 to 64 foot candles at the solutions surface under a photoperiod of 16 hours of light and 8 hours of darkness. The water had a total hardness and total alkalinity ranges as calcium carbonate of 36 to 38 mg/L and 28 to 30 mg/L respectively. The pH, dissolved oxygen concentration and temperature were measured at 0, 24, 48 (aged and new solutions), 72, and 96 hours of exposure in each test aquarium. The fish were fed a commercial prepared fish food diet ad libitum daily, except during the 48 hours prior to test initiation. The fish were not fed during definitive test. Based on the results of preliminary testing, nominal concentrations for the definitive study were 0.022, 0.037, 0.061, 0.10 and 0.17 mg a.i/L. The high concentration approximated the solubility limit of the compound as determined in a concurrent analytical study. One test aquarium was maintained for each treatment level and the controls. Each aquarium contained 10 fish. Test solutions were renewed at 48 hours of exposure. All aquaria were examined at 0 hour and following 24, 48, 72, and 96 hours of exposure.[1]
Type of test:	Static Renewal
Species:	Rainbow Trout (Oncorhynchus mykiss)
Mean Total Length:	43 mm (range 38 to 54 mm)

Mean Wet Weight: 0.70 g (range 0.43 to 1.2 g)

Number of fish: 10 fish per treatment level and the controls.

Test Concentrations: 0.022, 0.037, 0.061, 0.10 and 0.17 mg a.i./L (nominal)

Exposure period: 96 h

Analytical monitoring: Concentrations of Tinuvin P measured in the exposure solutions during the 96-hour static-renewal exposure of rainbow trout (Oncorhynchus mykiss) is shown in table below.

Nominal Concentration (mg a.i./L)	**Measured Concentration (mg a.i./L)**			
	0- Hour[a]	**48-Hour[a] Renewal**	**Mean[b] of New Solutions**	**96-Hour[c]**
Control	< 0.0053 (NA)	<0.0048 (NA)	NA	<0.0051 (NA)
Solvent Control	< 0.0053 (NA)	<0.0048 (NA)	NA	<0.0051 (NA)
0.022	0.021 (95)	0.018 (82)	0.019	0.0038 (17)
0.037	0.034 (91)	0.033 (89)	0.033	0.0085 (23)
0.061	0.069 (110)	0.054 (88)	0.062	0.0099 (16)
0.10	0.14 (140)	0.085 (85)	0.11	0.019 (19)
0.17	0.16 (92)	0.15(86)	0.15	0.035 (20)

[a] Freshly prepared solution
[b] Mean measured concentrations calculated from the 0- and 48- hour new solutions.
[c] Aged solutions, i.e. at study termination

GLP: Yes

Year: 2004

Results: At test termination (96 hours), no mortality or adverse effects were observed in any treated or

the control animals. Since no concentration tested resulted in $\geq$ 50% mortality, the 96-hour LC_{50} value was empirically estimated to be >0.17 mg a.i/L, the highest nominal concentration tested. The No-Observed-Effect Concentration (NOEC) was determined to be 0.17 mg a.i/L. The highest nominal concentration that produced 0% mortality was 0.17% mg a.i/L. Further testing to define the LC_{50} was not performed since the highest nominal concentration tested (0.17 mg a.i/L) corresponded to the water solubility of the test substance.

Remarks: This study was assigned a reliability code of 1a (GLP guideline study) according the criteria established by Klimisch *et al* (1997).[2]

Reference: [1]Tinuvin P – Acute Toxicity to Rainbow Trout (Oncorhynchus mykiss) Under Static-Renewal Conditions. Study No. 13658.6247, Springborn Smithers Laboratories, 15 January 2004.

[2] Klimisch, H.J., Andreae, M and Tillman, U. A systemic approach for evaluating the quality of experimental toxicological and ecotoxicological data. *Regulatory Toxicology and Pharmacology*. 25:1-5, 1997.

Table 1. Summary Table For CAS No. 2440-22-4

PHYSICAL/CHEMICAL ELEMENTS	DATE	RESULTS	FULFILLS REQUIREMENT
Melting Point	1989	131 - 133 ^{o}C (measured)	Yes
Boiling Point	2000	225 ^{o}C (measured)	Yes
Vapour Pressure	2000	7.94 x 10^{-8} mm Hg (*)	Yes
Partition Coefficient	2000	log P = 4.2 (measured)	Yes
Water Solubility	2003	0.173 mg/L (experimental-measured)	Yes
ENVIRONMENTAL FATE AND PATHWAYS ELEMENTS			
Photodegradation	2000	For reaction with hydroxyl radical, predicted rate constant = 92.5 x 10^{-12} cm^3/molecule-sec predicted half-life = 1.39 h (*)	Yes
Stability in Water	2000	Low solubility makes testing impractical. EPIWIN model will not calculate for this structure.	No
Fugacity	2000	Predicted distribution using Level III fugacity model Air 3.1 % Water 4.9 % Soil 87.3 % Sediment 4.6 % Persistence = 2757 h	Yes
Biodegradation	1989	Not biodegradable (measured) 11 mg/L: 0% after 28 days 20.1 mg/L: 2% after 28 days	Yes
ECOTOXICITY ELEMENTS			
Acute Toxicity to Fish	1984	Zebra fish (Brachydanio rerio): LC_{50} (96 h) > 100 mg a.i./L (nominal) NOEC (96 h) =100 mg a.i/L (nominal)	Yes
	2003	Rainbow Trout (Oncorhynchus mykiss): LC_{50} (96 h) > 0.17 mg a.i/L NOEC (96 h) > 0.17 mg a.i/L	Yes
Toxicity to Aquatic Plants		No data	No[1]
Acute Toxicity to Aquatic Invertebrates	1988	EC_0 (24 h) > 58 mg/L (nominal) EC_{50} (24 h) > 1000 mg/L (nominal) EC_{100} (24 h) > 1000 mg/L (nominal)	Yes

[1] Low toxicity to algae may be extrapolated from testing with other compounds in this category.

* Estimated Value using EPIWIN Model (Syracuse Research Corporation, 2000)

Table 1. (CONTINUED)

HEALTH ELEMENTS	DATE	RESULTS	FULFILLS REQUIREMENT
Acute Toxicity	1978	Rat: LD_{50} (Oral) > 10,000 mg/kg	Yes
	1975	Rat: LC_{50} (Inhalation, 4 h) > 1420 mg / m^3	Yes
Genetic Toxicity in vivo	1975	Mouse: No evidence of dominant lethal effects (single gavage dose of 1000 or 3000 mg/kg). No effect on mating ratio, implantations, or embryonic death.	Yes
	1977	Chinese hamster: Nonmutagenic in somatic mutation assay (exposed by gavage 500, 1000, or 2000 mg/kg/day for 2 days)	Yes
	1981	Chinese hamster: Nonmutagenic in somatic mutation assay (exposed by gavage 500, 1000, or 2000 mg/kg/day for 2 days)	Yes
Genetic Toxicity in vitro	1982	Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 10, 30, 90, 270 and 810 μg/0.1 mL)	Yes
Repeated Dose Toxicity	1981	90 Day (Dog): NOEL = 1000 ppm	Yes
Reproductive Toxicity		No effect on reproductive organs in repeat dose or chronic testing	Yes
Developmental Toxicity/Teratogenicity:	1965	Rat: Not teratogenic NOEL = 1000 mg/kg	Yes
	1965	Mouse: Not teratogenic NOEL = 1000 mg/kg	Yes
Lifetime Carcinogenicity	1978	No evidence of carcinogenicity after 24 months exposure to the following dietary concentrations Mouse: 0, 5, 50, 500 ppm Rat: 0, 100, 300, 1000, 3000 ppm	Yes

Table 2. Summary of Available Data for Phenolic Benzotriazole Category

SIDS Test	**CAS 2440-22-4** 2-(2-Hydroxy-5-methylphenyl)benzo-triazole Molecular Weight: 225.25	**CAS 3147-75-9** 2-(2-Hydroxy-5-tert-octylphenyl)benzo-triazole Molecular Weight: 323.44	**CAS 25973-55-1** 2-(2-Hydroxy-3,5-di-tert-amylphenyl) benzotriazole Molecular weight: 351.50	**CAS 70321-86-7** 2-(2H-Benzotrialzol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol Molecular Weight: 447.58
Acute Mammalian	LD50 >10,000 mg/kg	LD50 >10,000 mg/kg	LD50 >2325 mg/kg	LD50 >7750 mg/kg
Repeat Dose	NOEL = 1000 ppm (Dog)	NOEL > 5,658 mg/kg/day (Rat)	NOEL < 100 ppm (Rat); <15 mg/kg (Dog)	NOEL = 50 ppm (Rat)
Point/Gene Mutation	Negative (Ames)	Negative (Ames)	Negative (Ames)	Negative (Ames)
Chromosomal Aberration	Negative (3 *in vivo* studies)	No Data	No Data	Negative (*in vivo*)
Development/ Teratogenicity	NOEL = 1000 mg/kg (Rat, Mouse)	No Data	No Data	NOEL = 3000 mg/kg (Rat)
Reproduction	No effects on reproductive organs in Repeat dose testing	No Data	No effects on reproductive organs in Repeat dose testing	No effects on reproductive organs in Repeat dose testing
Carcinogenicity	No evidence of carcinogenicity in the rat or mouse (2 year Tests)	No Data	No Data	No Data

	2440-22-4	3147-75-9	25973-55-1	70321-86-7
Acute Fish	LC50 > 100 ppm (1988) LC50 > 0.173 mg/L (2004) [1]	LC50 > 100 ppm	LC50 > 100 ppm	LC50 > 67 ppm
Acute Daphnia	EC50 > 1,000 ppm	EC50 = 15 ppm	EC50 >100 ppm	EC50 > 91 ppm
Algae Growth Inhibition	No Data [2]	EC50 >100 ppm	EC50 > 10 ppm	EC50 > 100 ppm
Photodegradation	T1/2 = 1.39 hours (*)	T1/2 = 4.02 h (*)	T1/2 = 8.1 h (*)	T1/2 = 1.06 h (*)
Water Stability / hydrolysis	No Data[3]	No Data	No Data	No Data[3]
Fugacity Calculation (*)	Air 3.1% Water 4.9% Soil 87.3% Sediment 4.6%	Air 4.0 x 10^{-5}% Water 3.5% Soil 44.6% Sediment 51.9%	Air 2.3 x 10^{-4}% Water 2.2% Soil 40.4% Sediment 57.5%	Air 0% Water 2.2% Soil 40.1% Sediment 57.7%
Biodegradation	Not readily biodegradable (measured)	Not readily biodegradable (measured)	Not readily biodegradable (measured)	Not readily biodegradable (measured)
Melting Point	131-133 ^{o}C (measured)	106 - 108 ^{o}C (measured)	80 - 83 ^{o}C (measured)	139-143 ^{o}C (measured)
Boiling Point	225 ^{o}C (measured)	N/A	477.8 ^{o}C (*)	599.8 ^{o}C (*)
Water Solubility	0.173 mg/L (measured)	< 1 mg/L (measured) 0.168 mg/L (*)	0.015 mg/L (*)	0.04 mg/L (measured) 0.0097 mg/L (*)
Log P	4.2 (measured)	6.2 (*)	7.3 (*)	> 6.5 (measured) 7.2 (*)
Vapor Pressure	7.94 x 10^{-8} mm Hg (*)	1.1 x 10^{-9} mm Hg (*)	1.93 x 10^{-10} mm Hg (*)	1.62 x 10^{-14} mm Hg (*)

[1] New testing at solubility limit

[2] Based on data from the other benzotriazoles in the category the EC50 is estimated to be > 100 ppm.

[3] The low water solubility of these compounds makes it impractical to conduct hydrolysis studies.

* Estimated Value using EPIWIN Model (Syracuse Research Corporation, 2000)