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OVERALL SUMMARY FOR TRIISOPROPYLBORATE

Summary

Triisopropylborate (TIPB) is a colorless, moisture-sensitive liquid. It has a melting point of -59°C, boiling point of 140°C, and density of 0.8251 g/cm^3 at 20°C. TIPB has a vapor pressure of 100 mm Hg at 25.5°C, water solubility of 0% (hydrolyzes), and an estimated log Kow of 0.83.

TIPB is unstable in water and hydrolyzes with sequential loss of isopropanol groups to the end products of boric acid (CAS Registry #10043-35-3) and isopropanol (CAS Registry #67-63-0). However, no reliable data for hydrolysis was available, therefore a hydrolytic stability test, generally following OECD Guideline 111 is recommended. Boric acid will form soluble salts with monovalent cations (e.g. $Na_2B_4O_7.10H_2O$, 6% in water) and insoluble salts with divalent cations (e.g. $CaB_4O_7.6H_2O$, almost insoluble in cold water) (Budavari, 1989). Isopropanol is water soluble. Isopropanol and boric acid have little tendency to bioaccumulate (estimated log BCF = 0.5). Isopropanol is readily biodegradable, while boric acid is not subject to biodegradation. TIPB is estimated to have a half-life of 10.55 hours in air. Moisture may shorten the half-life in air. Emission to dry soil may result in a moderate soil half-life in the absence of moisture input, because of greater stability in the absence of moisture. Mackay Level III fugacity model, assuming equal emissions to air, water, and soil, predicts that TIPB will occupy mainly the water, with a lesser amount occupying the soil, little occupying air, and virtually none occupying sediment.

Since TIPB hydrolyzes, its aquatic toxicity potential is expected to be that of its hydrolysis products, isopropanol and boric acid. Isopropanol is of low concern for aquatic toxicity. Isopropanol has 96-hour LC_{50}s in fathead minnows and mysid shrimp of 9640-10,400 mg/L and 4050 mg/L, respectively. In another study, the 24-hour EC_{50} for daphnids was determined to be 159,000 µmol/L (29,906 mg/L). The 16-day log NOEC for growth and the log EC_{50} for reproduction in *Daphnia magna* were 3.37 µmol/L (0.63 mg/L) and 4.73 µmol/L (0.89 mg/L), respectively. Isopropanol had very low toxicity to green algae with a 5-day algistatic concentration of 54,294 ppm.

Boric acid is also of low concern for acute aquatic toxicity to fish with 96-hour LC_{50}s of >100 to 725 mg/L. Boric acid had a 48-hour LC_{50} in *Daphnia* of 133 mg/L, an 8-day EC_{50} *in Ceriodaphnia dubia* of >100 mg/L, and a 21-day LC_{50} in *Daphnia magna* of 52.2 mg/L. In another study with *Daphnia magna*, the 14-day NOEL was approximately 14 mg/L. The 7-day NOEC for boron using *Lemna minor* L. was >20 mg/L.

TIPB possesses very low to slight acute toxicity with an oral LD_{50} in rats and mice of 8126 mg/kg and 2500 mg/kg, respectively. TIPB was neither a skin irritant nor a skin sensitizer when tested in guinea pigs, and produced no to mild eye irritation when tested in rabbits.

No data are available to evaluate the potential repeated dose, reproductive, or developmental effects of TIPB. Therefore, a combined repeated dose toxicity study with the

reproduction/developmental toxicity screening test, following OECD Guideline 422, is recommended.

TIPB was negative in *Salmonella typhimurium* when tested in the *in vitro* bacterial reverse mutation assay. Since no information regarding chromosome aberrations was available, an *in vitro* chromosome aberration study, following OECD Guideline 473, is recommended.

Human Exposure

TIPB is manufactured at one DuPont facility. TIPB has been sold to 4 customers for commercial applications. Potential applications for TIPB use are pharmaceutical organic synthesis, lubricant additives, and as precursor material for creating Suzuki coupling reagents in the pharmaceutical market. Two customers who also produce TIPB also purchase TIPB for resale.

The potential for exposure is the greatest during shutdown work and loading and unloading. The site can have 2000 personnel working (construction, contractor, and plant employees). The areas where the substance is manufactured will have 4 operators during normal operations and 14 to 32 people during a shutdown or major construction activity. The site has effective safety, health, and environmental practices and procedures in addition to engineering controls, environmental controls, and personal protective equipment to control exposure. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities, are available in the event of an occupation exposure.

Individuals handling TIPB should wear coverall chemical splash goggles. A face shield should be worn where the possibility exists for face contact due to splashing or spraying of material. NIOSH approved respiratory protection should be worn, as appropriate. Where there is potential for skin contact, impervious gloves, apron, pants, and jacket should be worn as appropriate.

DuPont practices Responsible Care and assesses the ability of potential customers to safely handle TIPB prior to commencing a commercial relationship. The Product Stewardship System works with customers to understand their applications and any issues associated with PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc), storage concerns, disposal requirements, and MSDS questions.

References for Summary

Budavari, S. (ed.) (1989). The Merck Index. An Encyclopedia of Chemicals, Drugs, and Biolgoicals, 11th ed., Merck and Co., Inc., Rahway, NJ.

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TEST PLAN FOR TRIISOPROPYLBORATE

Triisopropylborate CAS No. 5419-55-6	**Data Available**	**Data Acceptable**	**Testing Required**
PHYSICAL/CHEMICAL CHARACTERISTICS			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
ENVIRONMENTAL FATE			
Photodegradation	Y	Y	N
Stability in Water	Y	N	Y
Transport (Fugacity)	Y	Y	N
Biodegradation	Y	Y	N
ECOTOXICITY			
Acute Toxicity to Fish	Y*	Y	N
Acute Toxicity to Invertebrates	Y*	Y	N
Acute Toxicity to Aquatic Plants	Y*	Y	N
MAMMALIAN TOXICITY			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	N	N	Y
Developmental Toxicity	N	N	Y
Reproductive Toxicity	N	N	Y
Genetic Toxicity Gene Mutations	Y	Y	N
Genetic Toxicity Chromosomal Aberrations	N	N	Y
* Data are available for hydrolysis products, boric acid and isopropyl alcohol.			