1,3-Propane Sultone

Safety Data Sheet

Division of Occupational Health and Safety
National Institutes of Health

WARNING!

This compound is absorbed through the intestinal tract. It is toxic, carcinogenic, mutagenic, and teratogenic. Avoid formation and breathing of aerosols.

Laboratory operations should be conducted in a fume hood, glove box, or ventilated cabinet.

Avoid skin contact: if exposed, wash with soap and water.

For eye exposure, irrigate immediately with large amounts of water. For ingestion, drink plenty of milk and water. Induce vomiting. For inhalation, remove victim promptly to clean air. Administer rescue breathing if necessary. Refer to physician.

In case of laboratory spill, wear protective clothing during cleanup. Avoid skin contact or breathing of aerosols. Use water to dissolve compound. Wash down area with soap and water. Dispose of waste solutions and materials appropriately.

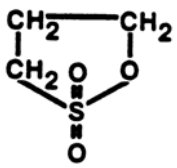
A. Background

1,3-Propane sultone (propane sultone) is a white crystalline solid below 31° C and colorless liquid above this temperature. It is stable in the absence of moisture but it is slowly hydrolyzed to a corrosive compound (3-hydroxyl-1-propanesulfonic acid) in the presence of water. It is toxic in rodents and irritating on contact with eyes and skin. Propane sultone is carcinogenic in rodents and mutagenic to plant and bacterial cells. It is chiefly used as a chemical intermediate in conferring water solubility to a variety of compounds.

B. Chemical and Physical Data

1. Chemical Abstract No.: 1120-71-4
2. Synonyms: Y-Propane sultone, 1,2-Oxathiolane, 2,2-dioxide (9CI), 3-Hydroxyl-1-propane sulphonic acid sulfone, 1-Propane sulfonic acid-3-hydroxyl-Y-sultone
3. Molecular formula, weight and structure:

   $C_3H_6O_3S$, 122.14,



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4. Density: solid, 1.51 g/cm³ at 20° C relative to water at 4° C; liquid, 1.392 g/cm³ at 40° C relative to water at 4° C.
5. Absorption spectroscopy: No data.
6. Volatility: Vapor pressure = 1 mm Hg at 100° C.
7. Solubility: Soluble in water (100 g/l) with slow decomposition.
8. Description, appearance: White odorless crystals below 31° C; colorless liquid above 31° C.
9. Boiling point: 112° C at 1.4 mm Hg.

   Melting point: 31° C.
10. Stability: Hydrolyzes in water to 3-hydroxyl-1-propanesulfonic acid. Half-life at 37° C in phosphate buffer, pH 7.4, 110 min.
11. Chemical reactivity: Reacts with carboxylic acids, primary amines, alcohols, mineral acids, and thiols to form addition compounds via the alcoholic hydroxyl group, which appears on hydrolysis.
12. Flash point: 158° C.
13. Autoignition temperature: No data.
14. Explosive limits in air: No data.

C. Fire, Explosion, and Reactivity Hazard Data

1. Propane sultone does not require special fire-fighting procedures or equipment and does not present unusual fire and explosion hazards.
2. A condition contributing to instability is the presence of moisture, which results in hydrolysis to free acid, which is highly corrosive to metals.
3. No other incompatibilities are known to exist.
4. Propane sultone does not require nonspark equipment.

D. Operational Procedures

The *NIH Guidelines for the Laboratory Use of Chemical Carcinogens* describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving propane sultone.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by propane sultone or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 911) for assistance. Wash surfaces with copious quantities of water. Glassware should be rinsed (in a hood) with water and washed with soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing propane sultone shall be disposed of in sinks or general refuse. Surplus propane sultone or chemical waste streams contaminated with propane sultone shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Non-chemical waste (*e.g.*, animal carcasses and bedding) containing propane sultone shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (*e.g.*, tissue cultures) containing

propane sultone shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (*e.g.*, absorbent bench top liners) minimally contaminated with propane sultone shall be handled as potentially infectious waste and packed for incineration, as above. Absorbent materials (*e.g.*, associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing propane sultone shall be handled in accordance with the NIH radioactive waste disposal system.

4. Storage: Store in sealed glass ampoules or screw-capped bottles or vials with Teflon cap liners. Avoid exposure to moisture and light. Refrigeration is recommended.

E. Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

1. Sampling: No data.
2. Separation and analysis: No specific methods have been reported. General methods for detection and estimation have been described, including colorimetric procedures using 4-picoline and o-dinitrobenzene as reagents (Sawicki and Sawicki, 1969) and the reaction with 4-(4-nitrobenzyl) pyridine (Preussmann *et al.*, 1969).

F. Biological Effects (Animal and Human)

1. Absorption: Propane sultone is absorbed by the digestive tract after ingestion and through the skin.
2. Distribution: Distributed after intestinal absorption to central and peripheral nervous systems, bone marrow, ear duct, liver, pancreas, ovaries, and mammary glands.
3. Metabolism and excretion: No data. In analogy with alkyl alkanesulfonates, one may assume that propane sultone reacts with the thiol groups of cysteine or cysteine-containing compounds with ring opening and excretion in the urine of the resulting S-propylsulfonic acid derivative of cysteine. Similar reactions may also be expected with primary amino and hydroxyl groups of peptides and proteins.
4. Toxic effects: The intraperitoneal LD_{50}s in the rat on subcutaneous, intravenous, and oral administration are 135, 210, and 350 mg/kg, respectively (Druckrey *et al.*, 1970), and the lowest lethal dose for dermal application in the mouse is 1,000 mg/kg (Doak *et al.*, 1976). No particular target organ has been identified. Eye and skin exposure can cause chemical burns, and propane sultone acts as a strong skin sensitizer in experimental animals. It has been reported that single skin exposures in humans produce a slow-healing burn (Ippen and Mathies, 1970). Animals exposed to 425 ppm of (heated) propane sultone by inhalation show delayed deaths, which indicate the possibility of cumulative toxic effects from repeated exposures.
5. Carcinogenic effects: Location of malignancies due to propane sultone appears to depend on mode of administration; skin application in mice results in tumors at the site of application (Doak *et al.*, 1976); oral or intravenous administration in rats produces tumors of the brain, kidney, and mammary glands (Druckrey *et al.*, 1970). Propane sultone is evidently transmitted across the placental barrier, since tumors of the brain, pancreas, and ovaries have been observed in the offspring of rats given a single intravenous dose during gestation.
6. Mutagenic and teratogenic effects: Propane sultone produces a positive response in the Ames test and induces mutations in yeast and rye cells. There are no data concerning its teratogenicity.

G. Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water or milk. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician. Observe for pulmonary irritation. Obtain ophthalmological consultation for eye exposure.

H. References

Doak, S.M.A., B.J.E. Simpson, P.F. Hunt, and D.E. Stevenson. 1976. The carcinogenic response in mice to the topical application of propane sultone to the skin. Toxicology 6:139-154.

Druckrey, H., H. Kruse, R. Preussmann, S. Ivankovic, C. Landschutz, and J. Gimmy. 1970. Carcinogenic alkylating substances. IV. 1,3-Propane sultone and 1,4-butane sultone. Z Krebsforsch 75:69-84.

Ippen, H., and V. Mathies. 1970. Protracted chemical burns (with special regard to those produced by epoxide and propane sultone). Berufsdermatosen 18:144-165.

Preussmann, R., H. Schneider, and F. Epple. 1969. Investigations for the determination of alkylating agents. II. The determination of different classes of alkylating agents with a modification of the color reaction with 4-(4-nitrobenzyl) pyridine (NBP). Arzneim Forsch 19:1059-1073.

Sawicki, E., and C.R. Sawicki. 1969. Analysis of alkylating agents: Application to air pollution. Ann NY Acad Sci 163:895-920.