Chemical Safety Data Sheet MSDS / SDS

1,3-propanesultone SDS

Revision Date:2024-04-25 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name: 1,3-propanesultone

CAS: 1120-71-4

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Dermal

Carcinogenicity, Category 1B

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H302 Harmful if swallowed
H312 Harmful in contact with skin
H350 May cause cancer

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P203 Obtain, read and follow all safety instructions before use.

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P317 Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P318 IF exposed or concerned, get medical advice.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	1,3-propanesultone
Common names and synonyms:	1,3-propanesultone
CAS number:	1120-71-4
EC number:	214-317-9
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Wear protective gloves when administering first aid. Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention if skin irritation occurs.

Following eye contact

Rinse with plenty of water for several minutes (remove contact lenses if easily possible). Refer for medical attention.

Following ingestion

Rinse mouth. Seek medical attention if you feel unwell.

Most important symptoms/effects, acute and delayed

Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin, respiratory system; [potential occupational carcinogen] Target Organs: Eyes, skin, respiratory system (NIOSH, 2016)

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: SMALL FIRE: Dry chemical, CO2 or water spray. LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

Specific hazards arising from the chemical

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Vacuum with specialist equipment (See Notes) or carefully sweep into sealable containers. If appropriate, moisten first to prevent dusting. If liquid: collect leaking liquid in sealable containers as far as possible. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Vacuum with specialist equipment (See Notes) or carefully sweep into sealable containers. If appropriate, moisten first to prevent dusting. If liquid: collect leaking liquid in sealable containers as far as possible. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. Chemical Carcinogens

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Dry. Well closed. Separated from food and feedstuffs.PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. Chemical Carcinogens

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: A3 (confirmed animal carcinogen with unknown relevance to humans).MAK: skin absorption (H); carcinogen category: 1; germ cell mutagen group: 3A

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use closed system.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Powder.
Colour:	Colourless.
Odour:	Foul odor above 31.11 deg C.
Melting point/freezing point:	31 °C.
Boiling point or initial boiling point and boiling range:	94 °C. Atm. press.:0.4 hPa.
Flammability:	Combustible Solid

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	171.5 °C. Atm. press.: 1 004 hPa.
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	< 1.
Kinematic viscosity:	no data available
Solubility:	10 % (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Pow = -2.86.
Vapour pressure:	0.003 hPa. Temperature: 20 °C. Remarks: Calculated from regression of the vapour pressure curve.; 0.005 hPa. Temperature: 25 °C. Remarks: Calculated from regression of the vapour pressure curve.; 0.089 hPa. Temperature: 50 °C. Remarks: Calculated from regression of the vapour pressure curve.
Density and/or relative density:	1.392. Temperature: 40 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

NIOSH considers propane sultone to be a potential occupational carcinogen.
Decomposes on heating. This produces toxic fumes including sulfur oxides. Reacts with moist air. This produces toxic 3-propane sulfonic acid.

Chemical stability

no data available

Possibility of hazardous reactions

PROPANE SULTONE reacts slowly with water to give 3-hydroxopropanesulfonic acid. This reaction may be accelerated by acid. May react with strong reducing agents to give toxic and flammable hydrogen sulfide.

Conditions to avoid

no data available

Incompatible materials

Evaporation of the residue after treatment of the thietane with hydrogen peroxide is liable to explode, and must be done in an open dish. This is probably because of formation of a 2 or 3-hydroperoxide derivative.

Hazardous decomposition products

When heated to decomposition propane sultone emits toxic fumes of SOx.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat - > 100 - < 200 mg/kg bw.

Inhalation: LC100 - rat - 2.14 mg/L air.

Dermal: LD15 - mouse (male/female) - 830 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

The Human Health Assessment Group in EPA's Office of Health and Environmental Assessment has evaluated 1,3-Propane sultone for carcinogenicity. According to their analysis, the weight-of-evidence for 1,3-Propane sultone is group B2, which is based on no evidence in humans and sufficient evidence in animals. As a group B2 chemical, 1,3-Propane sultone is considered as probably carcinogenic to humans.

Reproductive toxicity

No information is available on the reproductive or developmental effects of 1,3-propane sultone in humans. In the offspring of pregnant rats given a single intravenous injection of 1,3-propane sultone during gestation, malignant neurogenic tumors and tumors of the pancreas and ovary were reported.

STOT-single exposure

The substance is irritating to the eyes and skin. The skin effects may appear after a latency period of a few hours.

STOT-repeated exposure

This substance is carcinogenic to humans. May cause genetic damage in humans.

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Leuciscus idus - 72.5 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 16 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - > 320 mg/L - 72 h.

Toxicity to microorganisms: EC10 - Pseudomonas putida - ca. 26 mg/L - 17 h.

Persistence and degradability

No data were located concerning the biodegradation of 1,3-propane sultone either in natural systems or in laboratory studies(SRC). Since 1,3-propane sultone rapidly hydrolyzes in water (1,2), biodegradation probably will not be a significant process in the environment(SRC).

Bioaccumulative potential

Since 1,3-propane sultone hydrolyzes rapidly in water(1,2), bioconcentration in aquatic organisms is not expected to be a significant process(SRC).

Mobility in soil

Since 1,3-propane sultone hydrolyzes rapidly in water(1,2), and presumably in moist soil(SRC), adsorption to soil is not expected to be a significant process(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2811 (For reference only, please check.)
IMDG: UN2811 (For reference only, please check.)
IATA: UN2811 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)
IMDG: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)
IATA: TOXIC SOLID, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

NEVER use a domestic-type vacuum cleaner to vacuum the substance, only use specialist equipment.Depending on the degree of exposure, periodic medical examination is suggested.Do NOT take working clothes home.