Chemical Safety Data Sheet MSDS / SDS

Benzenethiol 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: Benzenethiol

CAS: 108-98-5

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 2, Oral
Acute toxicity - Category 2, Dermal

Skin irritation, Category 2
Acute toxicity - Category 1, Inhalation
Reproductive toxicity, Category 2
Specific target organ toxicity – single exposure, Category 3
Specific target organ toxicity – single exposure, Category 2
Specific target organ toxicity – repeated exposure, Category 1
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H300 Fatal if swallowed
H310 Fatal in contact with skin
H315 Causes skin irritation
H319 Causes serious eye irritation
H330 Fatal if inhaled
H335 May cause respiratory irritation
H361 Suspected of damaging fertility or the unborn child
H372 Causes damage to organs through prolonged or repeated exposure
H400 Very toxic to aquatic life
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P262 Do not get in eyes, on skin, or on clothing.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P203 Obtain, read and follow all safety instructions before use.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P320 Specific treatment is urgent (see ... on this label).
P318 IF exposed or concerned, get medical advice.
P319 Get medical help if you feel unwell.
P308+P316 IF exposed or concerned: Get emergency medical help immediately.
P391 Collect spillage.

Storage

P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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:	Benzenethiol
Common names and synonyms:	Benzenethiol

CAS number:	108-98-5
EC number:	203-635-3
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Marked potential for causing eye changes. May cause death (EPA, 1998)

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Sulfur and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Solid streams of water may be ineffective. Use foam, dry chemical, or carbon dioxide. Phenyl mercaptan

Specific hazards arising from the chemical

When heated to decomposition or on contact with acids, it emits toxic fumes of sulfur oxides. May be ignited by heat, sparks or flames. Container may explode in heat of fire. Vapor explosion and poison hazard indoors, outdoors or in sewers. Unstable, oxidizes in air. Avoid contact with acids. (EPA, 1998)

Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Environmental considerations: Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./ Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash, cement powder, or commercial sorbents. Phenyl mercaptan

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. 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

Separated from strong oxidants, strong acids and food and feedstuffs.Conditions for safe storage, including any incompatibilities: Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.1 ppm as TWA; (skin)

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 safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Water-white liquid
Odour:	Repulsive, penetrating, garlic-like odor, especially when impure
Melting point/freezing point:	-14.93 °C.
Boiling point or initial boiling point and boiling range:	169.1 °C.
Flammability:	Class II Combustible Liquid: Fl.P. at or above 100°F and below 140°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	50°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	Feebly acidic
Kinematic viscosity:	no data available
Solubility:	0.08 % at 77° F (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 2.52
Vapour pressure:	1.4 mm Hg (20 °C)

Density and/or relative density:	1.08 g/cm3. Temperature:20 °C.
Relative vapour density:	3.8 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. Decomposes on contact with acids. This produces toxic fumes of sulfur oxides. Reacts with strong oxidants.

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Flammable liquidPHENYL MERCAPTAN reacts with acids to generate toxic fumes of oxides of sulfur. [Lewis, 3rd ed., 1993, p. 1021]. Reacts exothermically with strong oxidizing agents.

Conditions to avoid

no data available

Incompatible materials

Strong acids & bases, calcium hypochlorite, alkali metals [Note: Oxidizes on exposure to air].

Hazardous decomposition products

When heated to decomposition or on contact with acids it emits toxic fumes of SOx /sulfur oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 46 mg/kg

Inhalation: LC50 Rat inhalation 33 ppm/4 hr

Dermal: no data available

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

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the nervous system.

STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis.

Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Oryzias latipes - 0.009 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 0.004 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 0.211 mg/L - 72 h.

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Using a Warburg respirometer and activated sludge inocula, thiophenol reached 30-42% of its theoretical BOD in 6 days(1). Using a Warburg respirometer and phenol or resorcinol-adapted yeast cells isolated from soil, oxidation of thiophenol occurred after a 10-30 min test lag(2). Thiophenol, present at 100 mg/L, reached 0% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(3).

Bioaccumulative potential

An estimated BCF of 20 was calculated in fish for thiophenol(SRC), using a log Kow of 2.52(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of thiophenol can be estimated to be 230(SRC). According to a classification scheme(2), this estimated Koc value suggests that thiophenol is expected to have moderate mobility in soil. The pKa of thiophenol is 6.62(3), indicating that this compound will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4). The sorption coefficient for thiophenol to snow was measured as log Ki 3.65 cu m/sq m(5).

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: UN2337 (For reference only, please check.)
IMDG: UN2337 (For reference only, please check.)
IATA: UN2337 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: PHENYL MERCAPTAN (For reference only, please check.)
IMDG: PHENYL MERCAPTAN (For reference only, please check.)
IATA: PHENYL MERCAPTAN (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: Yes
IMDG: Yes
IATA: Yes

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

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/

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any