

Chemical Safety Data Sheet MSDS / SDS

Benzothiazole-2-thiol SDS

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

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|-----------|------------|------------|------------|------------|------------|------------|------------|
| Section 1 | Section 2 | Section 3 | Section 4 | Section 5 | Section 6 | Section 7 | Section 8 |
| Section 9 | Section 10 | Section 11 | Section 12 | Section 13 | Section 14 | Section 15 | Section 16 |

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

Product name: Benzothiazole-2-thiol
CAS: 149-30-4

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**

Skin sensitization, Category 1
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H317 May cause an allergic skin reaction

H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P273 Avoid release to the environment.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P391 Collect spillage.

Storage

none

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: | Benzothiazole-2-thiol |
| Common names and synonyms: | Benzothiazole-2-thiol |
| CAS number: | 149-30-4 |
| EC number: | 205-736-8 |
| Concentration: | 100% |

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

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.

Most important symptoms/effects, acute and delayed

SYMPTOMS: Symptoms of exposure to this compound may include allergic contact dermatitis. Skin contact may also lead to sensitization. Eye contact can cause irritation. **ACUTE/CHRONIC HAZARDS:** This compound may be harmful by inhalation, ingestion or skin absorption. It is very irritating to the eyes. When heated to decomposition or upon contact with acid or acid fumes, it emits highly toxic fumes of carbon monoxide, carbon dioxide, sulfur oxides and nitrogen oxides. (NTP, 1992)

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. Aromatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

Special protective actions for fire-fighters

Use water spray, dry powder, foam, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: face shield and particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. 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. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Personal precautions, protective equipment and emergency procedure: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. PREVENT DISPERSION OF DUST. Closed system, dust explosion-proof electrical equipment and lighting. 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 acids. Conditions for safe storage, including any incompatibilities: Keep container tightly closed in a dry and well-ventilated place.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

MAK: (inhalable fraction): 4 mg/m³; carcinogen category: 3B; sensitization of skin (SH); pregnancy risk group: C

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.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

| | |
|---|--|
| Physical state: | Solid. Crystalline. |
| Colour: | Yellow. |
| Odour: | Disagreeable odor |
| Melting point/freezing point: | 180 - 182 °C. |
| Boiling point or initial boiling point and boiling range: | 64°C/4mmHg |
| Flammability: | Combustible. Gives off irritating or toxic fumes (or gases) in a fire. |
| Lower and upper explosion limit/flammability limit: | no data available |
| Flash point: | 200 °C. |
| Auto-ignition temperature: | 628°C |
| Decomposition temperature: | no data available |
| pH: | no data available |
| Kinematic viscosity: | no data available |
| Solubility: | less than 1 mg/mL at 66° F (NTP, 1992) |
| Partition coefficient n-octanol/water: | log Pow = 2.42. |

| | |
|----------------------------------|---|
| Vapour pressure: | < 0 hPa. Temperature:25 °C. |
| Density and/or relative density: | 1.42 g/cm ³ . Temperature:20 °C. |
| Relative vapour density: | no data available |
| Particle characteristics: | no data available |

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic and irritating fumes (sulfur oxides, nitrogen oxides). Reacts with acids and acid fumes. This produces toxic and irritating fumes (sulfur oxides, nitrogen oxides).

Chemical stability

no data available

Possibility of hazardous reactions

2-MERCAPTOBENZOTHAZOLE is incompatible with strong oxidizing agents. Also incompatible with acids and acid fumes (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

on contact with acid or acid fumes it emits toxic /oxides of sulfur and oxides of nitrogen/.

Hazardous decomposition products

When heated to decomp ... it emits toxic /oxides of sulfur and oxides of nitrogen/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 3 800 mg/kg bw. Remarks: Clinical signs: reduced appetite and activity, increased weakness, collapse and death.

Inhalation: LC50 - rat (male/female) - > 1 270 mg/L air.

Dermal: LD50 - rabbit (male/female) - > 7 940 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

Cancer Classification: Group C Possible Human Carcinogen

Reproductive toxicity

no data available

STOT-single exposure

The substance may be irritating to the eyes.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. See Notes. This substance is probably carcinogenic to humans.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oncorhynchus mykiss* (previous name: *Salmo gairdneri*) - 0.73 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 0.71 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 0.5 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge - 3 301 mg/L - 3 h. Remarks: Respiration rate.

Persistence and degradability

AEROBIC: Several biodegradation studies with 2-mercaptobenzothiazole using an activated sludge seed inoculum indicate little or no biodegradation(1-4). 2-Mercaptobenzothiazole, present at 100 mg/L, reached only 2.5% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test indicating the compound is not readily biodegradable(1). It has been suggested that at the concentrations used in these studies, 56-100 ppm, 2-mercaptobenzothiazole is toxic to the microorganisms in the sludge(5). A more detailed study indicated that inhibitory effects occur between 20 and 50 ppm of 2-mercaptobenzothiazole(5). When the sludge is well acclimated and the concentrations low enough, 2-mercaptobenzothiazole may completely biodegrade forming 2-benzothiazolesulfonate or dibenzothiazole-2,2-disulfide, depending on conditions(5). In a screening test comparable to OECD Method 301B (CO₂ evolution), 2-mercaptobenzothiazole, present at 17-18 mg/L, reached only 1-5% degradation after 35 days of incubation which classified the compound as not inherently biodegradable(6). Another CO₂ evolution study determined <1% degradation after 28 days using adapted activated sludge and an initial 2-mercaptobenzothiazole concentration of 23.8 mg/L(6). Partial degradation of 2-mercaptobenzothiazole was found in laboratory-scale fed-batch systems using activated sludge inoculum taken from rubber chemicals wastewater treatment plants(6).

Bioaccumulative potential

A BCF of <8 was measured in fish for 2-mercaptobenzothiazole(SRC), using carp (*Cyprinus carpio*) which were exposed over a 6-week period(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The K_{oc} of 2-mercaptobenzothiazole was measured as 677, 326 and 1360 in California sandy loam, California clay loam and

California sandy soil respectively(1). The Koc of 2-mercaptobenzothiazole was measured as 2130, 3560 and 2590 in three different sediments(1). The Koc of 2-mercaptobenzothiazole was measured as 915, 863, 1429 and 1829 in Drummer silty clay loam, Spinks sandy loam, Ray silt loam and Lintonia sandy loam soil respectively(1). According to a classification scheme(2), these estimated Koc values suggest that 2-mercaptobenzothiazole is expected to have moderate to slight mobility in soil. The pKa of 2-mercaptobenzothiazole is 7.03(1), 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(3).

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: UN3077 (For reference only, please check.)

IMDG: UN3077 (For reference only, please check.)

IATA: UN3077 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

IATA: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 9 (For reference only, please check.)

IMDG: 9 (For reference only, please check.)

IATA: 9 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (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

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

Do NOT take working clothes home. Isolate contaminated clothing by sealing in a bag or other container. Anyone who has shown skin sensitization due to this substance should avoid all further contact.

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