Chemical Safety Data Sheet MSDS / SDS

Di(benzothiazol-2-yl) disulphide 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: Di(benzothiazol-2-yl) disulphide

CAS: 120-78-5

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

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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:	Di(benzothiazol-2-yl) disulphide
Common names and synonyms:	Di(benzothiazol-2-yl) disulphide
CAS number:	120-78-5
EC number:	204-424-9
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 include skin and eye irritation. ACUTE/CHRONIC HAZARDS: This compound is a potential eye and skin irritant. When heated to decomposition it emits very toxic fumes of oxides of carbon, nitrogen and sulfur. (NTP, 1992)

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

Absorption, Distribution and Excretion

To determine the metabolic disposition of (l4)C-2-mercaptobenzothiazole (MBT) and (14)C-2-mercaptobenzothiazole disulfide (MBTS) male and female rats were dosed topically. Topical doses were 36.1 ug/animal for (14)C-MBT and 33.6 ug/animal for (14)C-MBTS. Although more MBT passed through the skin than MBTS and although relative to rats, guinea pigs absorbed a greater percentage of the dose (33.4% compared to 16.1-17.5% of the MBT and 12.2% compared to 5.94-7.87% for MBTS) the disposition of radioactivity derived from the two compounds was similar. Washing of the skin removed more of the radioactivity from guinea pigs than from rats. For both sexes of rats dosed iv with (14)C-MBT 0.602 mg/kg) or (14)C-MBTS 0.571 mg/kg) disposition of the compounds was similar. In 72 hr, 90.9-101% of the dose appeared in the urine and 3.79-15.1% in the feces. At this time a small portion of the administered radioactivity (1.52-1.96% of the dose) remained associated with erythrocytes. Oral dosing of rats for 14 days with unlabeled MBT (0.510 mg/kg/day) prior to a single dose of (14)C-MBT (0.503 mg/kg) or with unlabeled MBTS (0.521 mg/kg/day) prior to a single dose of (14)C-MBTS (0.730 mg/kg). For both sexes disposition of the compounds was similar. At 96 hr after dosing a small portion of the administered radioactivity (1.20-1.69% of the dose) remained associated with erythrocytes most of which was bound to the membranes. For both compounds and sexes 60.8-101% of the radioactivity administered appeared in the urine and 3.46-9.99% in the feces in 96 hr. At the time only trace amounts of radioactivity remained in tissues other than blood. Of these tissues thyroid contained the highest concentration. In the urine there was a detectable MBT or MBTS but there were two metabolites one of which was identified as a thioglucuronide derivative of MBT. The other was possibly a sulfonic acid derivative of MBT. In conclusion there were similarities in absorption, distribution, and metabolism of (14)C-MBT and (14)C-MBTS in rats and in guinea pigs, indicating that (14)C-MBTS was readily converted to (14)C-MBT.

SECTION 5: Firefighting measures

Suitable extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. A water spray may also be used. (NTP, 1992)

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

Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. PREVENT DISPERSION OF DUST. Prevent deposition 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

Materials which are toxic as stored or which can decompose into toxic components...should be stored in a cool well ventilated place, out of the direct rays of the sun, away from areas of high fire hazard, and should be periodically inspected. incompatible materials should be isolated...

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

MAK: sensitization of skin (SH)

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:	PHYSICAL DESCRIPTION: Cream to light yellow powder. (NTP, 1992)
Colour:	PALE YELLOW NEEDLES FROM BENZENE
Odour:	ODORLESS
Melting point/freezing point:	-108°C(lit.)
Boiling point or initial boiling point and boiling range:	65°C(lit.)
Flammability:	Combustible.

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	-15°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 0.1 mg/mL at 70° F (NTP, 1992)
Partition coefficient n-octanol/water:	4.5
Vapour pressure:	0mmHg at 25°C
Density and/or relative density:	1.5
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic and corrosive gases including carbon oxides, nitrogen oxides and sulfur oxides.

Chemical stability

no data available

Possibility of hazardous reactions

2,2'-DITHIOBISBENZOTHIAZOLE is incompatible with strong oxidizers. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition, such materials can evolve highly toxic fumes containing so(x). sulfur compd

SECTION 11: Toxicological information

Acute toxicity

Oral: no data available

Inhalation: no data available

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 may be irritating to the eyes.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. See Notes.

Aspiration hazard

Evaporation at 20°C is negligible; a nuisance-causing concentration of airborne particles can, however, be reached quickly.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

In an aerobic closed bottle screening study using activated sludge and soil inoculum, 2,2'-dibenzothiazyl disulfide had a 2 week theoretical BOD of 0.8%(1).

Bioaccumulative potential

Using a flow-through test system, 6-week BCFs for 2,2'-dibenzothiazyl disulfide of 1.0-7.2 and 1.4-51 were measured for concentrations of 0.2 mg/L and 0.02 mg/L, respectively, for carp(1). These experimental BCF values suggest that bioconcentration

in aquatic organisms is not expected to be an important fate process(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indexes, the Koc for 2,2'-dibenzothiazyl disulfide can be estimated to be about 755,000(1). The Koc for 2,2'-dibenzothiazyl disulfide can be estimated to be about 10,960 based on an estimated water solubility of 0.187 mg/L at 25 deg C and a regression derived equation(2). According to a suggested classification scheme(3), these estimated Koc values suggest that 2,2'-dibenzothiazyl disulfide is immobile in soil.

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.2-Mercaptobenzothiazole (MBT, see ICSC #1183) a substance closely related to MBTS, is classified by IARC for its carcinogenicity.Anyone who has shown skin sensitization due to this substance should avoid all further contact.