

Chemical Safety Data Sheet MSDS / SDS

2-(Thiocyanatomethylthio)benzothiazoleRevision Date:2025-06-14 Revision Number:1

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

Product name : 2-(Thiocyanatomethylthio)benzothiazole
CBnumber : CB9752494
CAS : 21564-17-0
EINECS Number : 244-445-0
Synonyms : TCMTB,Benthiazole

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral
Skin irritation, Category 2
Eye irritation, Category 2
Skin sensitization, Category 1
Acute toxicity - Category 2, Inhalation
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

Label elements**Pictogram(s)**

Signal word : Danger

Hazard statement(s)

H302 Harmful if swallowed
H315 Causes skin irritation

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H330 Fatal if inhaled

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.

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

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

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

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.

P273 Avoid release to the environment.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

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

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

P332+P317 If skin irritation occurs: Get medical help.

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

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P320 Specific treatment is urgent (see ... on this label).

P391 Collect spillage.

Storage

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name : 2-(Thiocyanatomethylthio)benzothiazole

Synonyms	: TCMTB,Benthiazole
CAS	: 21564-17-0
EC number	: 244-445-0
MF	: C9H6N2S3
MW	: 238.35

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

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 and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

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. Esters and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Use water spray, powder, foam, carbon dioxide.

Specific Hazards Arising from the Chemical

Combustible. Liquid formulations containing organic solvents may be flammable. Gives off irritating or toxic fumes (or gases) in a fire. Risk of fire and explosion if formulations contain flammable/explosive solvents.

Advice for firefighters

Use water spray, powder, foam, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. 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. Do NOT let this chemical enter the environment.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. 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. Do NOT let this chemical enter the environment.

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. 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 food and feedstuffs. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure 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

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

Information on basic physicochemical properties

Physical state	REDDISH VISCOUS LIQUID WITH PUNGENT ODOUR.
Colour	Oil
Odour	Pungent
Melting point/freezing point	<-10 deg C
Boiling point or initial boiling point and boiling range	405.6°C at 760 mmHg
Flammability	Combustible. Liquid formulations containing organic solvents may be flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	199.1°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water, 125 mg/L at 24 deg C
Partition coefficient n-octanol/water	log Kow = 3.23 at 20 deg C
Vapour pressure	8.65E-07mmHg at 25°C
Density and/or relative density	1.47 g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating. This produces toxic fumes including hydrogen cyanide, nitrogen oxides and sulfur oxides.

Chemical stability

no data available

Possibility of hazardous reactions

Decomposes on heating. This produces toxic fumes including hydrogen cyanide, nitrogen oxides and sulfur oxides.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of ... /sulfur oxides & nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 1,590 mg/kg
- 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 is corrosive to the eyes. The substance is irritating to the skin.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: /*Lepomis macrochirus*/ (Bluegill sunfish); Concentration: 0.047 ppm for 96 hr /60% formulation (Busan 72)/

/Conditions of bioassay not specified

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: *Daphnia magna* (Water Flea) age <24 hr; Conditions: freshwater, flow through; Concentration: 23 ug/L for 48 hr (95% confidence interval: 20-26 ug/L); Effect: intoxication, immobilization /80% purity

Toxicity to algae: EC50; Species: *Pseudokirchneriella subcapitata* (Green Algae); Conditions: freshwater, static, 25 deg C; Concentration: 39 ug/L for 30 hr; Effect: population abundance /100% purity

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: 2-(Thiocyanomethylthio)benzothiazole, 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 classifying the compound as not readily biodegradable(1). By contrast, thiocyanic acid, (2-benzothiazolylthio) methyl ester, at an initial concentration of 42 umol/L, was 95% degraded in 9 to 12 days using a mixed culture pilot plant designed for treatment of tannery wastes; 2-(methylthio)benzothiazole was the main product(2). Using OECD Method 301B (CO2 Evolution Modified Sturm Test), 96% of initial 2-(thiocyanomethylthio)benzothiazole degraded by day 28(3); however, it took >10 days for the degradation to increase from 10 to 60%, thereby classifying the compound as not readily biodegradable under the conditions of the test(3). Soil samples were incubated in the dark with the test compound at 25 deg C for 58 days; a soil aerobic metabolism half-life of 1.4 days was reported(3).

Bioaccumulative potential

Using carp (*Cyprinus carpio*) which were exposed over an 8-week period, a BCF range was of <14-20 and <153 to 268 was measured for 2-(thiocyanomethylthio)benzothiazole at concentrations of 2 and 0.2 ug/L, respectively(1). Using bluegill sunfish (*Lepomis macrochirus*) and a 28-day exposure period, BCF values of 44 and 184 were determined in the fillet and whole fish respectively(2). According to a classification scheme(3), BCF values of <30 are low, 30-100 are moderate and from 100 to 1,000 are high(SRC).

Mobility in soil

The adsorption of 2-(thiocyanomethylthio)benzothiazole was measured in five different soil types (sand, sandy loam, silt loam, clay and clay loam) with resulting Koc values ranging from 282 to 7896(1). Two soil adsorption studies conducted using OECD guidelines in four soil types determined Koc values of 633, 1,730, 2,060 and 2,270(2). According to a classification scheme(3), these Koc values suggest that 2-(thiocyanomethylthio)benzothiazole is expected to have moderate to no mobility 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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

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: II (For reference only, please check.)

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

IATA: II (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

Not 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?pagelD=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

If the substance is formulated with solvent(s) also consult the card(s) (ICSC) of the solvent(s). Carrier solvent may enhance the skin absorption. Carrier solvents used in commercial formulations may change physical and toxicological properties.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.