

# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

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## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** Benzothiazole-2-thiol

### 1.2 Other means of identification

**Product number** -  
**Other names** mercaptobenzothiazole; AG 63; 2(3H)-Benzothiazolethione

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.  
**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Yien Chemical Technology Co., Ltd  
**Address** Building 6, 28 Yingong Road, Fengxian District, Shanghai  
Chemical Industry Zone, Shanghai, 201400, China  
**Telephone** +86-400-133-2688

### 1.5 Emergency phone number

**Emergency phone number** +86-400-133-2688  
**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

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## SECTION 2: Hazard identification

### 2.1 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

### 2.2 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.

<b>Response</b>	<p>P272 Contaminated work clothing should not be allowed out of the workplace.</p> <p>P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...</p> <p>P273 Avoid release to the environment.</p> <p>P302+P352 IF ON SKIN: Wash with plenty of water/...</p> <p>P333+P317 If skin irritation or rash occurs: Get medical help.</p> <p>P321 Specific treatment (see ... on this label).</p> <p>P362+P364 Take off contaminated clothing and wash it before reuse.</p> <p>P391 Collect spillage.</p>
<b>Storage</b>	none
<b>Disposal</b>	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.

### 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

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

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## SECTION 4: First-aid measures

### 4.1 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.

### 4.2 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)

### 4.3 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

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## **SECTION 5: Fire-fighting measures**

### **5.1 Suitable extinguishing media**

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

### **5.2 Specific hazards arising from the chemical**

This chemical is combustible. (NTP, 1992)

### **5.3 Special protective actions for fire-fighters**

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

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## **SECTION 6: Accidental release measures**

### **6.1 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.

### **6.2 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.

### **6.3 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.

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## **SECTION 7: Handling and storage**

### **7.1 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.

### **7.2 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.

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Occupational Exposure limit values**

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

#### **Biological limit values**

no data available

### **8.2 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.

### 8.3 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

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## SECTION 9: Physical and chemical properties and safety characteristics

<b>Physical state</b>	Solid. Crystalline.
<b>Colour</b>	Yellow.
<b>Odour</b>	Disagreeable odor
<b>Melting point/freezing point</b>	180 - 182 °C.
<b>Boiling point or initial boiling point and boiling range</b>	64°C/4mmHg
<b>Flammability</b>	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
<b>Lower and upper explosion limit/flammability limit</b>	no data available
<b>Flash point</b>	200 °C.
<b>Auto-ignition temperature</b>	628°C
<b>Decomposition temperature</b>	no data available
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	no data available
<b>Solubility</b>	less than 1 mg/mL at 66° F (NTP, 1992)
<b>Partition coefficient n-octanol/water</b>	log Pow = 2.42.
<b>Vapour pressure</b>	< 0 hPa. Temperature:25 °C.
<b>Density and/or relative density</b>	1.42 g/cm <sup>3</sup> . Temperature:20 °C.
<b>Relative vapour density</b>	no data available
<b>Particle characteristics</b>	no data available

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## SECTION 10: Stability and reactivity

### 10.1 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).

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

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

## 10.4 Conditions to avoid

no data available

## 10.5 Incompatible materials

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

## 10.6 Hazardous decomposition products

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

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## 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.

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## SECTION 12: Ecological information

### 12.1 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.

### 12.2 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 (CO<sub>2</sub> 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 CO<sub>2</sub> 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).

### 12.3 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).

### 12.4 Mobility in soil

The Koc 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).

### 12.5 Other adverse effects

no data available

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## SECTION 13: Disposal considerations

### 13.1 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.

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## SECTION 14: Transport information

### 14.1 UN Number

ADR/RID: UN3077 (For reference only, please check.)

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

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

### 14.2 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.)
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### 14.3 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.)
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### 14.4 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.)
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### 14.5 Environmental hazards

ADR/RID: Yes	IMDG: Yes	IATA: Yes
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### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

## SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Benzothiazole-2-thiol	Benzothiazole-2-thiol	149-30-4	205-736-8
<b>European Inventory of Existing Commercial Chemical Substances (EINECS)</b>			Listed.
<b>EC Inventory</b>			Listed.
<b>United States Toxic Substances Control Act (TSCA) Inventory</b>			Listed.
<b>China Catalog of Hazardous chemicals 2015</b>			Not Listed.
<b>New Zealand Inventory of Chemicals (NZIoC)</b>			Listed.
<b>Philippines Inventory of Chemicals and Chemical Substances (PICCS)</b>			Listed.
<b>Vietnam National Chemical Inventory</b>			Listed.
<b>Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)</b>			Listed.
<b>Korea Existing Chemicals List (KECL)</b>			Listed.

## SECTION 16: Other information

#### Information on revision

<b>Creation Date</b>	July 15, 2019
<b>Revision Date</b>	July 15, 2019

#### 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](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.

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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*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 damage resulting from handling or from contact with the above product.*