

## SAFETY DATA SHEET

Version 6.7  
Revision Date 07/25/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Mercaptobenzothiazole

Product Number : 63730

Brand : Aldrich

Index-No. : 613-108-00-3

CAS-No. : 149-30-4

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Skin sensitization (Category 1), H317

Short-term (acute) aquatic hazard (Category 1), H400

Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Warning

Hazard Statements

H317

May cause an allergic skin reaction.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P261

Avoid breathing dust.

P272

Contaminated work clothing must not be allowed out of the workplace.

P273

Avoid release to the environment.

P280

Wear protective gloves.

P302 + P352

IF ON SKIN: Wash with plenty of soap and water.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P363

Wash contaminated clothing before reuse.

P391

Collect spillage.

P501

Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : 2-Benzothiazolethiol

Formula :  $C_7H_5NS_2$

Molecular weight : 167.25 g/mol

CAS-No. : 149-30-4

EC-No. : 205-736-8

Index-No. : 613-108-00-3

| Component                    | Classification                                                                                                                     | Concentration |
|------------------------------|------------------------------------------------------------------------------------------------------------------------------------|---------------|
| <b>benzothiazole-2-thiol</b> |                                                                                                                                    |               |
|                              | Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H317, H400, H410<br>M-Factor - Aquatic Acute: 1<br>M-Factor - Aquatic Chronic: 1 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Sulfur oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed. Dry.

Air sensitive.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

| Component             | CAS-No.  | Value                                 | Control parameters  | Basis                                               |
|-----------------------|----------|---------------------------------------|---------------------|-----------------------------------------------------|
| benzothiazole-2-thiol | 149-30-4 | TWA                                   | 5 mg/m <sup>3</sup> | USA. Workplace Environmental Exposure Levels (WEEL) |
|                       | Remarks  | Skin<br>Dermal Sensitization Notation |                     |                                                     |

## 8.2 Exposure controls

### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

### Personal protective equipment

#### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

#### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented. required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

|                                                 |                                                                                          |
|-------------------------------------------------|------------------------------------------------------------------------------------------|
| a) Appearance                                   | Form: crystalline<br>Color: light yellow                                                 |
| b) Odor                                         | unpleasant                                                                               |
| c) Odor Threshold                               | No data available                                                                        |
| d) pH                                           | No data available                                                                        |
| e) Melting point/freezing point                 | Melting point/ range: 177 - 181 °C (351 - 358 °F) - lit.                                 |
| f) Initial boiling point and boiling range      | > 260 °C > 500 °F - Regulation (EC) No. 440/2008, Annex, A.2<br>- Decomposes on heating. |
| g) Flash point                                  | 200 °C (392 °F) - closed cup - ISO 1523                                                  |
| h) Evaporation rate                             | No data available                                                                        |
| i) Flammability (solid, gas)                    | No data available                                                                        |
| j) Upper/lower flammability or explosive limits | Lower explosion limit: 15 %(V)                                                           |
| k) Vapor pressure                               | No data available                                                                        |
| l) Vapor density                                | No data available                                                                        |
| m) Density                                      | 1.42 g/cm <sup>3</sup> at 20 °C (68 °F)                                                  |
| Relative density                                | No data available                                                                        |
| n) Water solubility                             | 0.118 g/l at 25 °C (77 °F)                                                               |
| o) Partition coefficient: n-octanol/water       | log Pow: 2.42 - Bioaccumulation is not expected.                                         |
| p) Autoignition temperature                     | does not ignite                                                                          |
| q) Decomposition temperature                    | No data available                                                                        |
| r) Viscosity                                    | No data available                                                                        |
| s) Explosive properties                         | Not classified as explosive.                                                             |
| t) Oxidizing properties                         | none                                                                                     |

### 9.2 Other safety information

Dissociation constant 7.03 at 20.5 °C (68.9 °F)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.  
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 3,800 mg/kg

Remarks: (ECHA)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

LC50 Inhalation - Rat - > 1,270 mg/m<sup>3</sup> - dust/mist

Remarks: (RTECS)

Symptoms: Irritation symptoms in the respiratory tract., Cough, Shortness of breath, After a latency period:, Inhalation may lead to the formation of oedemas in the respiratory tract.

LD50 Dermal - Rabbit - male and female - > 7,940 mg/kg

Remarks: (ECHA)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

Remarks: (ECHA)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 24 h

Remarks: (ECHA)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

**Germ cell mutagenicity**

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Intraperitoneal

Result: negative

Remarks: (ECHA)

**Carcinogenicity**

IARC: 2A - Group 2A: Probably carcinogenic to humans (benzothiazole-2-thiol)

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: DL6475000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Headache

Nausea

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Vomiting

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

|                                                                       |                                                                                                                      |
|-----------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                                      | flow-through test LC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - 0.73 mg/l - 96 h<br>(OECD Test Guideline 203)  |
| Toxicity to daphnia and other aquatic invertebrates                   | EC50 - <i>Daphnia magna</i> (Water flea) - 0.71 mg/l - 48 h<br>(OECD Test Guideline 202)                             |
| Toxicity to algae                                                     | ErC50 - <i>Pseudokirchneriella subcapitata</i> - 0.5 mg/l - 72 h<br>(OECD Test Guideline 201)                        |
| Toxicity to bacteria                                                  | static test EC50 - activated sludge - 3,301 mg/l - 3 h<br>(OECD Test Guideline 209)                                  |
| Toxicity to fish(Chronic toxicity)                                    | flow-through test NOEC - <i>Oncorhynchus mykiss</i> (rainbow trout) - 0.041 mg/l - 89 d<br>(OECD Test Guideline 210) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | EC50 - <i>Daphnia magna</i> (Water flea) - 0.33 mg/l - 21 d<br>(OECD Test Guideline 211)                             |
|                                                                       | NOEC - <i>Daphnia magna</i> (Water flea) - 0.08 mg/l - 21 d<br>(OECD Test Guideline 211)                             |

### 12.2 Persistence and degradability

|                  |                                                            |
|------------------|------------------------------------------------------------|
| Biodegradability | aerobic - Exposure time 14 d<br>(OECD Test Guideline 301C) |
|------------------|------------------------------------------------------------|

### 12.3 Bioaccumulative potential

|                 |                                                                                    |
|-----------------|------------------------------------------------------------------------------------|
| Bioaccumulation | <i>Cyprinus carpio</i> (Carp) - 42 d<br>at 25 °C - 0.1 mg/l(benzothiazole-2-thiol) |
|                 | Bioconcentration factor (BCF): < 0.8<br>(OECD Test Guideline 305C)                 |

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

### DOT (US)

Not dangerous goods

### IMDG

UN number: 3077    Class: 9    Packing group: III    EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (benzothiazole-2-thiol)

Marine pollutant : yes

Marine pollutant : no

### IATA

UN number: 3077    Class: 9    Packing group: III

Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (benzothiazole-2-thiol)

### Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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## SECTION 15: Regulatory information

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

## **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : The following components are subject to reporting levels established by SARA Title III, Section 313:

benzothiazole- 149-30-4 >= 90 - <= 100 %  
2-thiol

## **Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

## **Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

## **US State Regulations**

### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **California Prop. 65**

WARNING: This product can expose you to chemicals including benzothiazole-2-thiol, which is/are known to the State of California to cause cancer. For more information go to [www.P65Warnings.ca.gov](http://www.P65Warnings.ca.gov).

### **The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information****Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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