

# • SAFETY DATA SHEET

Version 6.5  
Revision Date 11/06/2025  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 3-Mercaptobenzoic acid  
Product Number : 451436  
Brand : Aldrich  
CAS-No. : 4869-59-4

### 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 number

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

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## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

Skin irritation : Category 2

Serious eye damage : Category 1  
Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

### Other hazards

None known.

### GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H315 Causes skin irritation.  
H318 Causes serious eye damage.  
H335 May cause respiratory irritation.

Precautionary statements : **Prevention:**  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear protective gloves/ eye protection/ face protection.

**Response:**  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P310 Immediately call a POISON CENTER/ doctor.  
P321 Specific treatment (see supplemental first aid instructions on this label).  
P332 + P313 If skin irritation occurs: Get medical advice/ attention.  
P362 Take off contaminated clothing and wash before reuse.

**Storage:**  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P405 Store locked up.

**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 4869-59-4

#### Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
3-Mercaptobenzoic acid	4869-59-4*	<= 100	-

\* Indicates that the identifier is a CAS No.

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### SECTION 4. FIRST AID MEASURES

General advice : Show this 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.

In case of eye contact : After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

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

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

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### SECTION 5. FIREFIGHTING MEASURES

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

Hazardous combustion products : Carbon oxides

Aldrich - 451436

Page 3 of 12

Sulphur oxides

- Specific extinguishing methods : No data available
- Further information : Suppress (knock down) gases/vapours/mists with a water spray jet.  
Prevent fire extinguishing water from contaminating surface water or the ground water system.
- Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

- 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.  
Advice for emergency responders:  
For personal protection see section 8.
- Environmental precautions : Do not let product enter drains.
- 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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Further information on storage conditions : Tightly closed.  
Dry.
- Storage class : 11, Combustible Solids
- Recommended storage temperature : Recommended storage temperature see product label.

Further information on storage stability : Air sensitive.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : 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.

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.

### Hand protection

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Full contact  
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.  
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)).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Tightly fitting safety goggles
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : solid
- Color : No data available
- Odor : Stench.
- Odor Threshold : No data available  
pH : No data available
- Melting point/ range : 291 - 297 °F / 144 - 147 °C  
Method: lit.
- Boiling point/boiling range : No data available
- Flash point : No data available
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Upper explosion limit /  
Upper flammability limit : No data available
- Lower explosion limit /  
Lower flammability limit : No data available
- Vapor pressure : No data available
- Relative vapour density : No data available

Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: log Pow: 1.917
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 154.19 g/mol
Particle characteristics	
Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: No data available
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Exposure to air may affect product quality. no information available
Incompatible materials	: Strong oxidizing agents
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

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

Remarks: No data available

#### Respiratory or skin sensitization

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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

No data available

#### Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

### 11.2 Additional Information

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

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **3-Mercaptobenzoic acid:**

Toxicity to fish : Remarks: No data available

### Persistence and degradability

#### Components:

##### **3-Mercaptobenzoic acid:**

Biodegradability : Remarks: No data available

### Bioaccumulative potential

#### Components:

##### **3-Mercaptobenzoic acid:**

Bioaccumulation : Remarks: No data available

Partition coefficient: n- : log Pow: 1.917  
octanol/water

### Mobility in soil

#### Components:

##### **3-Mercaptobenzoic acid:**

Stability in soil : Remarks: No data available

### Other adverse effects

#### Components:

##### **3-Mercaptobenzoic acid:**

Additional ecological : No data available  
information

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : 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

### International Regulations

#### IATA-DGR

UN/ID No. : UN 3335  
Proper shipping name : Aviation regulated solid, n.o.s.  
(3-Mercaptobenzoic acid)  
Class : 9  
Packing group : III  
Labels : Class 9 - Miscellaneous dangerous substances and  
articles  
Packing instruction (cargo : 956  
aircraft)  
Packing instruction : 956  
(passenger aircraft)

#### IMDG-Code

Not regulated as a dangerous good

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

#### National Regulations

##### 49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

#### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
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**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### US State Regulations

##### Massachusetts Right To Know

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

Aldrich - 451436

Page 10 of 12

### **Pennsylvania Right To Know**

3-Mercaptobenzoic acid

4869-59-4

### **New Jersey Right To Know**

3-Mercaptobenzoic acid

4869-59-4

### **California Prop. 65**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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

TSCA : Product contains substance(s) not listed on 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**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the

Aldrich - 451436

Page 11 of 12

European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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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