

SAFETY DATA SHEET

Version 4.10
Revision Date 09/12/2018
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Benzyl mercaptan

Product Number : B25401

Brand : Aldrich

CAS-No. : 100-53-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 2), H330

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (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

Danger

Hazard statement(s)

H227 Combustible liquid.

H302 Harmful if swallowed.

H330 Fatal if inhaled.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stench.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : α -Toluenethiol
 α -Tolyl mercaptan

Formula : C_7H_8S
Molecular weight : 124.20 g/mol
CAS-No. : 100-53-8
EC-No. : 202-862-5

Hazardous components

Component	Classification	Concentration
Toluene-α-thiol		
	Flam. Liq. 4; Acute Tox. 4; Acute Tox. 2; Aquatic Acute 1; Aquatic Chronic 1; H227, H302, H330, H410	90 - 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

- 5.1 Extinguishing media**
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
Unsuitable extinguishing media
Do NOT use water jet.
- 5.2 Special hazards arising from the substance or mixture**
No data available
- 5.3 Advice for firefighters**
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information**
Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.
- 6.2 Environmental precautions**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
- 6.3 Methods and materials for containment and cleaning up**
Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.
- 6.4 Reference to other sections**
For disposal see section 13.

7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
- 7.3 Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- 8.1 Control parameters**
Components with workplace control parameters
Contains no substances with occupational exposure limit values.
Hazardous components without workplace control parameters
- 8.2 Exposure controls**
Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

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

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.40 mm

Break through time: 60 min

Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.70 mm

Break through time: 480 min

Material tested:Butoject® (KCL 898)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

required when vapours/aerosols are generated. Filter B (acc. to DIN 3181) for inorganic gases and vapours

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|-------------------------------------|
| a) Appearance | Form: liquid |
| b) Odour | stinging |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point: -29.2 °C (-20.6 °F) |
| f) Initial boiling point and boiling range | 194 - 195 °C (381 - 383 °F) - lit. |
| g) Flash point | No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Lower explosion limit: 1 %(V) |
| k) Vapour pressure | 0.5 hPa (0.4 mmHg) at 20 °C (68 °F) |
| l) Vapour density | No data available |

m) Relative density	1.058 g/cm ³ at 25 °C (77 °F)
n) Water solubility	practically insoluble
o) Partition coefficient: n-octanol/water	log Pow: 2.48 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong bases, Strong oxidizing agents, Strong acids

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 493 mg/kg

Remarks: (RTECS)

absorption

LC50 Inhalation - Mouse - 4 h - 0.9 mg/l

Remarks: (External MSDS)

Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation

Remarks: (External MSDS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation

Remarks: (External MSDS)

Respiratory or skin sensitisation

Sensitisation test: - Guinea pig

Result: negative

Remarks: (External MSDS)

Germ cell mutagenicity

No data available

Ames test

Result: negative

(Lit.)

Carcinogenicity

Carcinogenicity - Mouse - Skin

Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Skin and Appendages: Other: Tumors.

Tumorigenic: Tumors at site or application.

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.

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard**Additional Information**

RTECS: Not available

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

Systemic effects:

After absorption of large quantities:

Cyanosis, muscular weakness, Shortness of breath, somnolence, Coma

Other information

The following applies to mercaptans in general: offensive odour.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

No data available

Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 0.15 mg/l - 48 h (OECD Test Guideline 202)
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12.2 Persistence and degradability

Biodegradability	Result: 40.7 % - Not readily biodegradable.
	Remarks: (External MSDS)

12.3 Bioaccumulative potential**12.4 Mobility in soil****12.5 Results of PBT and vPvB assessment**

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

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

Discharge into the environment must be avoided.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2810 Class: 6.1 Packing group: II
Proper shipping name: Toxic, liquids, organic, n.o.s. (Toluene- α -thiol)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2810 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (Toluene- α -thiol)
Marine pollutant: yes

IATA

UN number: 2810 Class: 6.1 Packing group: II
Proper shipping name: Toxic liquid, organic, n.o.s. (Toluene- α -thiol)

15. REGULATORY INFORMATION

SARA 302 Components

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

SARA 313 Components

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.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

Toluene- α -thiol	CAS-No. 100-53-8	Revision Date 1993-04-24
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Pennsylvania Right To Know Components

Toluene- α -thiol	CAS-No. 100-53-8	Revision Date 1993-04-24
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California Prop. 65 Components

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

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity

Flam. Liq.	Flammable liquids
H227	Combustible liquid.
H302	Harmful if swallowed.
H330	Fatal if inhaled.
H400	Very toxic to aquatic life.

Further information

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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. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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