SAFETY DATA SHEET

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

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 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)

Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 2), H330
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: 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/ vapors/ 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

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>benzyl mercaptan</td>
<td>Flam. Liq. 4; Acute Tox. 4; Acute Tox. 2; Aquatic Acute 1; Aquatic Chronic 1; H227, H302, H330, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Synonyms:
- α-Toluenethiol
- α-Tolyl mercaptan

Formula: C<sub>7</sub>H<sub>8</sub>S
Molecular weight: 124.20 g/mol
CAS-No.: 100-53-8
EC-No.: 202-862-5
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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. 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) 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
Sulfur oxides
Combustible.
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
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage class (TRGS 510): 6.1A: 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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters
Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.
8.2 Exposure controls

**Appropriate engineering controls**
Change contaminated clothing. Preventive skin protection recommended. Wash hands 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**
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 EC 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**
protective clothing

**Respiratory protection**
required when vapours/aerosols 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**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: liquid</td>
</tr>
<tr>
<td>b) Odor</td>
<td>stinging</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing</td>
<td>Melting point: -29.2 °C (-20.6 °F)</td>
</tr>
<tr>
<td>f) Initial boiling point</td>
<td>194 - 195 °C 381 - 383 °F - lit.</td>
</tr>
</tbody>
</table>
and boiling range

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>g) Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>Lower explosion limit: 1 % (V)</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>0.5 hPa at 20 °C (68 °F)</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>m) Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>practically insoluble</td>
</tr>
<tr>
<td>o) Partition coefficient: n-octanol/water</td>
<td>log Pow: 2.48 at 25 °C (77 °F) - Bioaccumulation is not expected.</td>
</tr>
<tr>
<td>p) Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>t) Oxidizing properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2 **Other safety information**
No data available

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**SECTION 10: Stability and reactivity**

10.1 **Reactivity**
Forms explosive mixtures with air on intense heating.

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
Strong acids

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
SECTION 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 sensitization**
Sensitisation test: - Guinea pig
Result: negative
Remarks: (External MSDS)

**Germ cell mutagenicity**
Test Type: Ames test
Result: negative
Remarks: (Lit.)

**Carcinogenicity**
IARC: No ingredient 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 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**

**Specific target organ toxicity - single exposure**

**Specific target organ toxicity - repeated exposure**

**Aspiration hazard**

11.2 Additional Information
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.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 0.15 mg/l - 48 h
(OECD Test Guideline 202)

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

Discharge into the environment must be avoided.
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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

**DOT (US)**
- UN number: 2810
- Class: 6.1
- Packing group: II
- Proper shipping name: Toxic, liquids, organic, n.o.s. (benzyl mercaptan)
- 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. (benzyl mercaptan)
- Marine pollutant: Yes

**IATA**
- UN number: 2810
- Class: 6.1
- Packing group: II
- Proper shipping name: Toxic liquid, organic, n.o.s. (benzyl mercaptan)

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

SECTION 16: Other information

**Further information**
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
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