SAFETY DATA SHEET

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

1.1 Product identifiers

Product name : Benzenethiol
Product Number : W361607
Brand : Aldrich
CAS-No. : 108-98-5

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 3), H226
- Acute toxicity, Oral (Category 2), H300
- Acute toxicity, Inhalation (Category 1), H330
- Acute toxicity, Dermal (Category 2), H310
- Skin irritation (Category 2), H315
- Serious eye damage (Category 1), H318
- Reproductive toxicity (Category 2), H361
- 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)
- H226 Flammable liquid and vapor.
- H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.
- H315 Causes skin irritation.
- H318 Causes serious eye damage.
- H361 Suspected of damaging fertility or the unborn child.
- H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)
- P201 Obtain special instructions before use.
- P202 Do not handle until all safety precautions have been read and understood.
- P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
- P233 Keep container tightly closed.
- P240 Ground/bond container and receiving equipment.
- P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
- P242 Use only non-sparking tools.
- P243 Take precautionary measures against static discharge.
- P260 Do not breathe mist or vapors.
- P262 Do not get in eyes, on skin, or on clothing.
- 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/ protective clothing/ eye protection/ face protection.
- P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
- P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
- P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
- P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
- P308 + P313 IF exposed or concerned: Get medical advice/ attention.
- P332 + P313 If skin irritation occurs: Get medical advice/ attention.
- P362 Take off contaminated clothing and wash before reuse.
- 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.
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>Synonyms</th>
<th>Phenyl mercaptan</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Thiophenol</td>
</tr>
<tr>
<td></td>
<td>Benzenethiol</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₆H₆S</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>110.18 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>108-98-5</td>
</tr>
<tr>
<td>EC-No.</td>
<td>203-635-3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>thiophenol</td>
<td>Flam. Liq. 3; Acute Tox. 2; Acute Tox. 1; Acute Tox. 2; Skin Irrit. 2; Eye Dam. 1; Repr. 2; Aquatic Acute 1; Aquatic Chronic 1; H226, H300, H330, H310, H315, H318, H361, H400, H410</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

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

If swallowed
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
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. Risk of explosion.
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
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class
Storage class (TRGS 510): 3: Flammable liquids

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>thiophenol</td>
<td>108-98-5</td>
<td>TWA</td>
<td>0.1 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Remarks Danger of cutaneous absorption</td>
</tr>
</tbody>
</table>
### 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). Tightly fitting safety goggles

#### 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- **Full contact**
  - Material: Viton®
  - Minimum layer thickness: 0.7 mm
  - Break through time: 480 min
  - Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

- **Splash contact**
  - Material: butyl-rubber
  - Minimum layer thickness: 0.7 mm
  - Break through time: 10 min
  - Material tested: Butoject® (KCL 898)

#### Body Protection
Flame retardant antistatic 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. Risk of explosion.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid
    Color: colorless

b) Odor Stench.

c) Odor Threshold No data available

d) pH No data available

e) Melting point/freezing point Melting point/range: -15 °C (5 °F) - lit.

f) Initial boiling point and boiling range 169 °C 336 °F - lit.

g) Flash point 50 °C (122 °F) - closed cup

h) Evaporation rate No data available

i) Flammability (solid, gas) No data available

j) Upper/lower flammability or explosive limits No data available

k) Vapor pressure 4.5 hPa at 40 °C (104 °F)
    1.9 hPa at 20 °C(68 °F)

l) Vapor density 3.8 - (Air = 1.0)

m) Density 1.073 g/cm3 at 25 °C (77 °F) - lit.
    Relative density No data available

n) Water solubility No data available

o) Partition coefficient: n-octanol/water No data available

p) Autoignition temperature No data available

q) Decomposition temperature No data available

r) Viscosity No data available

s) Explosive properties No data available

t) Oxidizing properties none

9.2 Other safety information

Relative vapor density 3.8 - (Air = 1.0)
SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

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

10.3 Possibility of hazardous reactions
A risk of explosion and/or of toxic gas formation exists with the following substances:
- Strong acids
- Hydrogen sulphide
- Increased reactivity with:
  - Strong oxidizing agents
  - Strong bases
  - Bases
  - Acids

10.4 Conditions to avoid
- Air
- Heating.

10.5 Incompatible materials
- Metals

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 - 46.2 mg/kg
- Behavioral: Coma.
- Respiratory disorder
- LC50 Inhalation - Rat - 4 h - 0.15 mg/l - vapor
  - Remarks: Lungs, Thorax, or Respiration: Respiratory stimulation.
  - Behavioral: Somnolence (general depressed activity).
  - Sense Organs and Special Senses (Nose, Eye, Ear, and Taste): Eye: Lacrimation.
  - (RTECS)
- LD50 Dermal - Rabbit - 134 mg/kg
  - Behavioral: Ataxia.
  - Cyanosis
  - (RTECS)
  - No data available

Skin corrosion/irritation
- Remarks: No data available
Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available
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
Some evidence of adverse effects on sexual function and fertility, and/or on development, based on animal experiments.

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: DC0525000
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:

Dizziness
Headache
Shortness of breath
Unconsciousness
agitation
Convulsions
Diarrhea
muscular weakness
Cyanosis
ataxia (impaired locomotor coordination)
Tremors

The following applies to mercaptans in general: offensive odour.
depressed respiration
Drowsiness
SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: semi-static test LC50 - *Oryzias latipes* (Japanese medaka) - 0.009 mg/l - 96 h (OECD Test Guideline 203)

- Toxicity to daphnia and other aquatic invertebrates: semi-static test EC50 - *Daphnia magna* (Water flea) - 0.004 mg/l - 48 h (OECD Test Guideline 202)

- Toxicity to algae: static test EC50 - *Pseudokirchneriella subcapitata* (green algae) - 0.211 mg/l - 72 h (OECD Test Guideline 201)

- Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity): NOEC - *Daphnia magna* (Water flea) - 0.002 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

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

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.
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.

SECTION 14: Transport information

DOT (US)
UN number: 2337  Class: 6.1I (3)  Packing group: I
Proper shipping name: Phenyl mercaptan
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: Hazard Zone B

IMDG
UN number: 2337  Class: 6.1 (3)  Packing group: I  EMS-No: F-E, S-D
Proper shipping name: PHENYL MERCAPTAN

IATA
UN number: 2337  Class: 6.1 (3)
Proper shipping name: Phenyl mercaptan
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

SECTION 15: Regulatory information

SARA 302 Components
thiophenol  CAS-No.  Revision Date
108-98-5  2007-07-01

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
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
thiophenol  CAS-No.  Revision Date
108-98-5  2007-07-01

Pennsylvania Right To Know Components
thiophenol  CAS-No.  Revision Date
108-98-5  2007-07-01
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 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.

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Version: 8.5    Revision Date: 06/06/2023    Print Date: 07/29/2023