1. PRODUCT AND COMPANY IDENTIFICATION

Product name: Thiophenol

Product Number: T32808

Brand: Aldrich

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

Telephone: +1 800-325-5832
Fax: +1 800-325-5052

Emergency Phone #: (314) 776-6555

Preparation Information: Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OMHA Hazards
Combustible Liquid, Highly toxic by inhalation, Highly toxic by ingestion, Highly toxic by skin absorption, Irritant

Other hazards which do not result in classification
Stench.

GHS Classification
Flammable liquids (Category 3)
Acute toxicity, Oral (Category 2)
Acute toxicity, Inhalation (Category 1)
Acute toxicity, Dermal (Category 2)
Serious eye damage (Category 1)

GHS Label elements, including precautionary statements

Pictogram

Signal word: Danger

Hazard statement(s)
H26 Flammable liquid and vapour.
H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled
H318 Causes serious eye damage.

Precautionary statement(s)
P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P264 Wash hands thoroughly after handling.
P280 Wear protective gloves/ eye protection/ face protection.
P284 Wear respiratory protection.
P302 + P350 IF ON SKIN: Gently wash with plenty of soap and water.
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 or doctor/physician.
HMIS Classification
   Health hazard: 4
   Flammability: 2
   Physical hazards: 0

NFPA Rating
   Health hazard: 4
   Fire: 2
   Reactivity Hazard: 0

Potential Health Effects
   Inhalation: May be fatal if inhaled. Causes respiratory tract irritation.
   Skin: May be fatal if absorbed through skin. Causes skin irritation.
   Eyes: Causes eye irritation.
   Ingestion: May be fatal if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

   Synonyms: Phenyl mercaptan, Benzenethiol
   Formula: C₆H₆S
   Molecular Weight: 110.18 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzenethiol</td>
<td></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>

4. 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
   Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

   If swallowed
   Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

   Suitable extinguishing media
   For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

   Special protective equipment for firefighters
   Wear self contained breathing apparatus for fire fighting if necessary.

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

6. ACCIDENTAL RELEASE MEASURES

   Use water spray to cool unopened containers.
Personal precautions
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.

Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

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.

Conditions for safe storage
Store in cool place. 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.

Store under inert gas. Air sensitive.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

<table>
<thead>
<tr>
<th>Components</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzenethiol</td>
<td>108-98-5</td>
<td>C</td>
<td>0.1 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.5 mg/m³</td>
<td></td>
</tr>
<tr>
<td>Remarks</td>
<td></td>
<td></td>
<td>15 minute ceiling value</td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td></td>
<td></td>
<td>0.1 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td>Upper Respiratory Tract &amp; skin irritation Anemia Danger of cutaneous absorption</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TWA</td>
<td></td>
<td></td>
<td>0.5 ppm</td>
<td>USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2 mg/m³</td>
<td></td>
</tr>
</tbody>
</table>

Personal protective equipment

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand 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.

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

Splash contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)
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.

**Eye protection**
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin and body protection**
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Hygiene measures**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### 9. PHYSICAL AND CHEMICAL PROPERTIES

#### Appearance
- **Form**: clear, liquid
- **Colour**: colourless

#### Safety data
- **pH**: no data available
- Melting point/freezing point: Melting point/range: -15 °C (5 °F) - lit.
- **Boiling point**: 169 °C (336 °F) - lit.
- **Flash point**: 50 °C (122 °F) - closed cup
- **Ignition temperature**: 450 °C (842 °F)
- **Auto-ignition temperature**: no data available
- **Lower explosion limit**: no data available
- **Upper explosion limit**: no data available
- **Vapour pressure**: 4.5 hPa (3.4 mmHg) at 40 °C (104 °F)
  1.9 hPa (1.4 mmHg) at 20 °C (68 °F)
- **Density**: 1.073 g/mL at 25 °C (77 °F)
- **Water solubility**: no data available
- **Partition coefficient: n-octanol/water**: no data available
- **Relative vapour density**: 3.8
  - (Air = 1.0)
- **Odour**: unpleasant
- **Odour Threshold**: no data available
- **Evaporation rate**: no data available

### 10. STABILITY AND REACTIVITY

**Chemical stability**
Stable under recommended storage conditions.

**Possibility of hazardous reactions**
no data available
**Conditions to avoid**
Heat, flames and sparks.

**Materials to avoid**
Do not store near acids., Strong bases, Strong oxidizing agents

**Hazardous decomposition products**
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides
Other decomposition products - no data available

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**11. TOXICOLOGICAL INFORMATION**

**Acute toxicity**

**Oral LD50**
LD50 Oral - rat - 46.2 mg/kg

**Inhalation LC50**
LC50 Inhalation - rat - 4 h - 33 ppm

**Dermal LD50**
LD50 Dermal - rabbit - 134 mg/kg

**Other information on acute toxicity**
no data available

**Skin corrosion/irritation**

**Serious eye damage/eye irritation**
Eyes - rabbit - Severe eye irritation

**Respiratory or skin sensitisation**
no data available

**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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

Reproductive toxicity - rat - Oral
Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Fertility: Litter size (e.g.; # fetuses per litter; measured before birth). Effects on Embryo or Fetus: Other effects to embryo.
Reproductive toxicity - rat - Oral
Maternal Effects: Other effects.

no data available

**Teratogenicity**
no data available

**Specific target organ toxicity - single exposure (Globally Harmonized System)**
no data available

**Specific target organ toxicity - repeated exposure (Globally Harmonized System)**
no data available

**Aspiration hazard**
no data available

**Potential health effects**

- **Inhalation**: May be fatal if inhaled. Causes respiratory tract irritation.
- **Ingestion**: May be fatal if swallowed.
- **Skin**: May be fatal if absorbed through skin. Causes skin irritation.
- **Eyes**: Causes eye irritation.

**Signs and Symptoms of Exposure**
Cough, Shortness of breath, Headache, Nausea, Vomiting

**Synergistic effects**
no data available

**Additional Information**
RTECS: DC0525000

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**12. ECOLOGICAL INFORMATION**

**Toxicity**
no data available

**Persistence and degradability**
no data available

**Bioaccumulative potential**
no data available

**Mobility in soil**
no data available

**PBT and vPvB assessment**
no data available

**Other adverse effects**
no data available

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**13. DISPOSAL CONSIDERATIONS**

**Product**
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**
Dispose of as unused product.

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**14. TRANSPORT INFORMATION**

**DOT (US)**
- UN number: 2337  
- Class: 6.1 (3)  
- Packing group: I

**Proper shipping name**: Phenyl mercaptan

**Reportable Quantity (RQ)**: 100 lbs

**Marine pollutant**: No

**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
Marine pollutant: No

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

15. REGULATORY INFORMATION

OSHA Hazards
Combustible Liquid, Highly toxic by inhalation, Highly toxic by ingestion, Highly toxic by skin absorption, Irritant

SARA 302 Components
The following components are subject to reporting levels established by SARA Title III, Section 302:

<table>
<thead>
<tr>
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<th>Revision Date</th>
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<td>108-98-5</td>
<td>2007-07-01</td>
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SARA 313 Components
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.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

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Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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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

Further information
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