

## SAFETY DATA SHEET

Version 4.7  
Revision Date 06/28/2016  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 4-Methylbenzenethiol

Product Number : T28525  
Brand : Aldrich

CAS-No. : 106-45-6

## 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)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

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

Eye irritation (Category 2A), H319

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 : Warning

Hazard statement(s)  
H319

Causes serious eye irritation.

Precautionary statement(s)

P264

Wash skin thoroughly after handling.

P280

Wear eye protection/ face protection.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Synonyms : 4-Mercaptotoluene

Aldrich - T28525

4-Methylthiophenol  
*p*-Toluenethiol  
*p*-Tolyl mercaptan  
*p*-Thiocresol

Formula : C<sub>7</sub>H<sub>8</sub>S  
Molecular weight : 124.20 g/mol  
CAS-No. : 106-45-6  
EC-No. : 203-399-1

#### Hazardous components

| Component              | Classification      | Concentration |
|------------------------|---------------------|---------------|
| <b>Toluene-4-thiol</b> |                     |               |
|                        | Eye Irrit. 2A; H319 | <= 100 %      |

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

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## 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. 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

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

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 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

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

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.

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Safety glasses with side-shields conforming to EN166 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, 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.

##### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**

Do not let product enter drains.

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**9. PHYSICAL AND CHEMICAL PROPERTIES****9.1 Information on basic physical and chemical properties**

|                                                 |                                                       |
|-------------------------------------------------|-------------------------------------------------------|
| a) Appearance                                   | Form: crystalline<br>Colour: beige                    |
| b) Odour                                        | unpleasant                                            |
| c) Odour Threshold                              | No data available                                     |
| d) pH                                           | No data available                                     |
| e) Melting point/freezing point                 | Melting point/range: 41 - 43 °C (106 - 109 °F) - lit. |
| f) Initial boiling point and boiling range      | 195 °C (383 °F) - lit.                                |
| g) Flash point                                  | 68 °C (154 °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) Vapour pressure                              | 13 hPa (10 mmHg) at 71 °C (160 °F)                    |
| l) Vapour density                               | No data available                                     |
| m) Relative density                             | No data available                                     |
| n) Water solubility                             | No data available                                     |
| o) Partition coefficient: n-octanol/water       | No data available                                     |
| 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

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**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

No data available

#### 10.5 Incompatible materials

Strong bases, Strong oxidizing agents

#### 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

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### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity

Inhalation: No data available

Dermal: No data available

LD50 Intraperitoneal - Mouse - 200 mg/kg

##### Skin corrosion/irritation

No data available

##### Serious eye damage/eye irritation

Irritating to eyes. Information given is based on data obtained from similar substances.

##### 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

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

No data available

##### Additional Information

RTECS: XT8925000

Nausea, Headache, Vomiting

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### 12. ECOLOGICAL INFORMATION

#### 12.1 Toxicity

No data available

**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 Other adverse effects**

No data available

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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

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: 3335      Class: 9

Proper shipping name: A Aviation regulated solid, n.o.s. (Toluene-4-thiol)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

**IMDG**

Not dangerous goods

**IATA**

UN number: 3335      Class: 9

Packing group: III

Proper shipping name: Aviation regulated solid, n.o.s. (Toluene-4-thiol)

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**15. REGULATORY INFORMATION****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**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.

**Pennsylvania Right To Know Components**

|                 | CAS-No.  | Revision Date |
|-----------------|----------|---------------|
| Toluene-4-thiol | 106-45-6 |               |

**New Jersey Right To Know Components**

|                 | CAS-No.  | Revision Date |
|-----------------|----------|---------------|
| Toluene-4-thiol | 106-45-6 |               |

**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.

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## 16. OTHER INFORMATION

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

|            |                                |
|------------|--------------------------------|
| Eye Irrit. | Eye irritation                 |
| H319       | Causes serious eye irritation. |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: |   |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 2 |
| Reactivity Hazard: | 0 |

### Further information

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### Preparation Information

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

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