

# SAFETY DATA SHEET

Version 6.7  
Revision Date 10/03/2021  
Print Date 11/27/2021

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

### 1.1 Product identifiers

Product name : Toluene-3,4-dithiol

Product Number : D129208

Brand : Aldrich

CAS-No. : 496-74-2

### 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

Not a hazardous substance or mixture.

### 2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

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

Stench.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : 'Dithiol'  
4-Methyl-1,2-benzenedithiol  
3,4-Dimercaptotoluene

Aldrich - D129208

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Formula : C<sub>7</sub>H<sub>8</sub>S<sub>2</sub>  
Molecular weight : 156.27 g/mol  
CAS-No. : 496-74-2  
EC-No. : 207-828-3

No components need to be disclosed according to the applicable regulations.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### **If inhaled**

After inhalation: fresh air.

#### **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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

### 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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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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 on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed. Dry.

#### Storage stability

Recommended storage temperature  
-20 °C

Handle and store under inert gas.

#### Storage class

Storage class (TRGS 510): 11: Combustible Solids

### 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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## 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. 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**

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: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (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 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.

### **Respiratory protection**

required when dusts 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**

- |  |   |
|--|---|
| a) Appearance                              | Form: powder<br>Color: white                        |
| b) Odor                                    | No data available                                   |
| c) Odor Threshold                          | No data available                                   |
| d) pH                                      | No data available                                   |
| e) Melting point/freezing point            | Melting point/range: 30 - 33 °C (86 - 91 °F) - lit. |
| f) Initial boiling point and boiling range | 135 - 137 °C 275 - 279 °F at 23 hPa - lit.          |
| g) Flash point                             | 113 °C (235 °F) - closed cup                        |
| h) Evaporation rate                        | No data available                                   |
| i) Flammability (solid,                    | No data available                                   |

	gas)	
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	1.179 g/mL 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	No data available

## 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.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 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

### 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

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### 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

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

### 11.2 Additional Information

RTECS: XT2275000

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

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## SECTION 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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## **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](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## **SECTION 14: Transport information**

#### **DOT (US)**

Not dangerous goods

#### **IMDG**

Not dangerous goods

#### **IATA**

UN number: 3335    Class: 9    Packing group: III  
Proper shipping name: Aviation regulated solid, n.o.s. (toluene-3,4-dithiol)

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## **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.

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

**Pennsylvania Right To Know Components**

toluene-3,4-dithiol

CAS-No.  
496-74-2

Revision Date

**New Jersey Right To Know Components**

toluene-3,4-dithiol

CAS-No.  
496-74-2

Revision Date

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**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](http://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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