

# SAFETY DATA SHEET

Version 6.7  
Revision Date 06/06/2024  
Print Date 07/13/2024

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

### 1.1 Product identifiers

Product name : 3,7-Dimethyl-3-octanol

Product Number : 309915  
Brand : Aldrich  
CAS-No. : 78-69-3

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 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  
Short-term (acute) aquatic hazard (Category 2), H401

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

## 2.2 GHS Label elements, including precautionary statements

Pictogram	none
Signal Word	Warning
Hazard Statements	
H227	Combustible liquid.
H401	Toxic to aquatic life.
Precautionary Statements	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

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### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms	:	Tetrahydrolinalool
Formula	:	C <sub>10</sub> H <sub>22</sub> O
Molecular weight	:	158.28 g/mol
CAS-No.	:	78-69-3
EC-No.	:	201-133-9

Component	Classification	Concentration
<b>3,7-Dimethyloctan-3-ol</b>		
	Flam. Liq. 4; Aquatic Acute 2; H227, H401	<= 100 %

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

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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**

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

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**

Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. 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 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.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### 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. 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.

#### Storage class

Storage class (TRGS 510): 10: Combustible liquids

### 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

not required

##### Respiratory protection

Not required; except in case of aerosol formation.

##### 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: liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	-23 °C (-9 °F) at 1,013 hPa - lit.
f) Initial boiling point and boiling range	71 - 73 °C 160 - 163 °F at 8 hPa - lit.
g) Flash point	76 °C (169 °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	0.111 hPa at 19.6 °C (67.3 °F)
l) Vapor density	5.46 - (Air = 1.0)
m) Density	0.826 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	0.32 g/l at 25 °C (77 °F)
o) Partition coefficient: n-octanol/water	log Pow: 3.3 at 20 °C (68 °F)
p) Autoignition temperature	360 °C (680 °F) at 1,013 hPa
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

Relative vapor density	5.46 - (Air = 1.0)
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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.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents, Acid chlorides, Acid anhydrides, Strong acids, Strong bases

### 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

LD50 Oral - Rat - male and female - 8,270 mg/kg  
LC0 Inhalation - Rat - male and female - 8 h - 0.885 mg/l - vapor

LD50 Dermal - Rabbit - > 5,000 mg/kg  
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

Tests on bacterial or mammalian cell cultures did not show mutagenic effects.  
Test system: *S. typhimurium*  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative

#### 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

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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**

Repeated dose toxicity - Rat - male and female - Oral - NOAEL (No observed adverse effect level) - 160 mg/kg

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**

Toxicity to fish                      semi-static test LC50 - Danio rerio (zebra fish) - 8.9 mg/l - 96 h  
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates                      Immobilization EC50 - Daphnia magna (Water flea) - 14.2 mg/l - 48 h  
(OECD Test Guideline 202)

Toxicity to algae                      Growth inhibition EC50 - Desmodesmus subspicatus (green algae) - 13.2 mg/l - 72 h  
(OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability                      aerobic - Exposure time 28 d  
Result: 60 - 70 % - Readily biodegradable.  
(OECD Test Guideline 301)

**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

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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.

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## SECTION 14: Transport information

#### DOT (US)

NA-Number: 1993 Class: NONE Packing group: III  
Proper shipping name: Combustible liquid, n.o.s. (3,7-Dimethyloctan-3-ol)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

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## SECTION 15: Regulatory information

#### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

#### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

#### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard

**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.



### **Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489).

### **Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

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

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

#### **The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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Version: 6.7

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