

# SAFETY DATA SHEET

Version 6.8  
Revision Date 08/06/2024  
Print Date 08/07/2024

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

### 1.1 Product identifiers

Product name : 1-Octanol

Product Number : 297887  
Brand : Sigma-Aldrich  
CAS-No. : 111-87-5

### 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  
Eye irritation (Category 2A), H319  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H227 Combustible liquid.  
 H319 Causes serious eye irritation.  
 H400 Very toxic to aquatic life.  
 H412 Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
 P264 Wash skin thoroughly after handling.  
 P273 Avoid release to the environment.  
 P280 Wear protective gloves/ 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.  
 P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.  
 P391 Collect spillage.  
 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 : Octyl alcohol  
 Capryl alcohol  
 Alcohol C8

Formula : C<sub>8</sub>H<sub>18</sub>O  
 Molecular weight : 130.23 g/mol  
 CAS-No. : 111-87-5  
 EC-No. : 203-917-6

Component	Classification	Concentration
<b>1-octanol</b>		
	Flam. Liq. 4; Eye Irrit. 2A; Aquatic Acute 1; Aquatic Chronic 3; H227, H319, H400, H412	<= 100 %

	M-Factor - Aquatic Acute: 1	
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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**

No data available

##### **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**

No data available

##### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides  
Combustible.

##### **5.3 Advice for firefighters**

No data available

##### **5.4 Further information**

No data available

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#### **SECTION 6: Accidental release measures**

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

For personal protection see section 8.

##### **6.2 Environmental precautions**

No data available

##### **6.3 Methods and materials for containment and cleaning up**

No data available

##### **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**

No data available

**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**

Component	CAS-No.	Value	Control parameters	Basis
1-octanol	111-87-5	TWA	50 ppm	USA. Workplace Environmental Exposure Levels (WEEL)

**8.2 Exposure controls****Personal protective equipment****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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

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Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 240 min

Material tested: KCL 720 Camapren®

**Respiratory protection**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented. 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**

Prevent product from entering drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |
|---|---|
| a) Appearance                                   | Form: clear, liquid<br>Color: colorless                   |
| b) Odor   | characteristic  |
| 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      | 196 °C 385 °F - lit.                                      |
| g) Flash point                                  | 86.5 °C (187.7 °F) at ca.101.5 hPa - ASTM D 93            |
| h) Evaporation rate                             | No data available   |
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | Lower explosion limit: 0.8 %(V)                           |
| k) Vapor pressure                               | 0.18 hPa at 25 °C (77 °F)                                 |
| l) Vapor density                                | No data available   |
| m) Density                                      | 0.827 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.           |
| Relative density                                | No data available   |
| n) Water solubility                             | 107 g/l at 23 °C (73 °F) - partly soluble                 |
| o) Partition coefficient: n-octanol/water       | log Pow: 3.5 at 23 °C (73 °F)                             |
| p) Autoignition temperature                     | ca.294 °C (ca.561 °F) at 1,013 hPa                        |
| q) Decomposition temperature                    | No data available   |
| r) Viscosity                                    | 5.584 mm <sup>2</sup> /s at 40 °C (104 °F) - ASTM D 445 - |

s) Explosive properties No data available

t) Oxidizing properties none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Acid chlorides

Acid anhydrides

Oxidizing agents

acids

halogen compounds

Risk of explosion with:

perchloric acid

perchlorates

### 10.4 Conditions to avoid

No data available

### 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

LD50 Oral - Rat - male and female - > 5,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 2,000 - 4,000 mg/kg

(OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation - 4 h

(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Buehler Test - Guinea pig

Result: negative

(US-EPA)

**Germ cell mutagenicity**

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vivo micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

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 on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

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 - Dermal - NOAEL (No observed adverse effect level) - 1,000 mg/kg

Repeated dose toxicity - Rat - male and female - Gavage - 28 Days - NOAEL (No observed adverse effect level) - > 1,000 mg/kg

Central nervous system depression, Nausea, Headache, Vomiting, narcosis  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 13.3 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.765 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 14 mg/l - 48 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - activated sludge - 350 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 0.26 mg/l - 33 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 1 mg/l - 21 d (OECD Test Guideline 211)

### 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d  
Result: 82.2 % - Readily biodegradable.  
(OECD Test Guideline 301B)

Ratio BOD/ThBOD 32 - 62 %

### 12.3 Bioaccumulative potential

Does not bioaccumulate.

### 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

No data available

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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. (1-octanol)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-octanol)

Marine pollutant : yes

Marine pollutant : no

### IATA

UN number: 3082 Class: 9 Packing group: III

Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (1-octanol)

### Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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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  
Acute Health Hazard  
Chronic Health 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.

## **US State Regulations**

### **Massachusetts Right To Know**

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

### **Pennsylvania Right To Know**

1-octanol

111-87-5

### **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**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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