

## SAFETY DATA SHEET

Version 6.5  
Revision Date 03/05/2024  
Print Date 03/06/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Octanol

Product Number : 95446

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

### 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

#### **General advice**

Show this material safety data sheet to the doctor in attendance.

#### **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. Call in ophthalmologist. Remove contact lenses.

#### **If swallowed**

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

### 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. Avoid substance contact. Ensure adequate ventilation. 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

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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

### 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

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)

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)).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 240 min

Material tested: KCL 720 Camapren®

#### Body Protection

protective clothing

#### 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

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: clear, liquid 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/mL 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**

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**

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**

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**

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

RTECS: RH6550000

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.

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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

#### 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. (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

#### 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

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

1-octanol

CAS-No.  
111-87-5

Revision Date  
1989-08-11

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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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