

## SAFETY DATA SHEET

Version 8.3  
Revision Date 12/01/2021  
Print Date 12/01/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Octene for synthesis

Product Number : 8.20928  
Catalogue No. : 820928  
Brand : Millipore  
CAS-No. : 111-66-0

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

Identified uses : Chemical for synthesis

**1.3 Details of the supplier of the safety data sheet**

Company : EMD Millipore Corporation  
400 Summit Drive  
BURLINGTON MA 01803  
UNITED STATES

Telephone : +1 800-645-5476

**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 2), H225  
Aspiration hazard (Category 1), H304  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

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

Danger

Hazard statement(s)  
H225

Highly flammable liquid and vapor.

H304	May be fatal if swallowed and enters airways.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P331	Do NOT induce vomiting.
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.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

Repeated exposure may cause skin dryness or cracking.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula	: C <sub>8</sub> H <sub>16</sub>
Molecular weight	: 112.22 g/mol
CAS-No.	: 111-66-0
EC-No.	: 203-893-7

Component	Classification	Concentration
<b>Oct-1-ene</b>	Flam. Liq. 2; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H304, H400, H410 M-Factor - Aquatic Acute: 1	<= 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

#### 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. 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

Nature of decomposition products not known.

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

### 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. Risk of explosion.

### **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 carefully 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. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

#### **Storage class**

Storage class (TRGS 510): 3: Flammable 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**

Component	CAS-No.	Value	Control parameters	Basis
Oct-1-ene	111-66-0	TWA	75 ppm	USA. Workplace Environmental Exposure Levels (WEEL)

## 8.2 Exposure controls

### Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. 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

#### Body Protection

Flame retardant antistatic protective clothing.

#### Respiratory protection

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. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>Color: colorless                                   |
| b) Odor   | benzine-like   |
| c) Odor Threshold                               | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | Melting point: -102 °C (-152 °F)                                   |
| f) Initial boiling point and boiling range      | No data available  |
| g) Flash point                                  | 8 °C (46 °F) - c.c.  |
| h) Evaporation rate                             | 1.3  |
| i) Flammability (solid, gas)                    | No data available  |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 6.8 %(V)<br>Lower explosion limit: 0.7 %(V) |
| k) Vapor pressure                               | 17.3 hPa at 20 °C (68 °F)  |
| l) Vapor density                                | 3.9  |

m) Density	0.72 g/cm <sup>3</sup> at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	practically insoluble
o) Partition coefficient: n-octanol/water	log Pow: 4.57 at 25 °C (77 °F) - (IUCLID), Potential bioaccumulation
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	0.38 mm <sup>2</sup> /s at 40 °C (104 °F) -
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

## 9.2 Other safety information

Relative vapor density	3.9
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 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  
 Strong acids  
 nitrates  
 chlorates  
 Peroxides

### 10.4 Conditions to avoid

Warming.

### 10.5 Incompatible materials

Bromine, Chlorine, Acids, Oxidizing agents, Humid air, Strong oxidizing agents

### 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 - > 5,000 mg/kg

Remarks: (IUCLID)

Millipore - 8.20928

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LC50 Inhalation - Rat - 4 h - 37.6 mg/l - vapor

Remarks: (IUCLID)

LD50 Dermal - Rabbit - > 2,000 mg/kg

Remarks: (IUCLID)

### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

### **Respiratory or skin sensitization**

Patch test: - Guinea pig

Result: Not a skin sensitizer.

(OECD Test Guideline 406)

### **Germ cell mutagenicity**

Test Type: Ames test

Result: negative

Remarks: (IUCLID)

Test Type: Ames test

Test system: *S. 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: inhalation (vapor)

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**

May be fatal if swallowed and enters airways.

## 11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 1,000 mg/kg

Prolonged or repeated exposure to skin causes defatting and dermatitis., Contact with eyes can cause:, Redness, Lachrymation, Blurred vision, Aspiration or inhalation may cause chemical pneumonitis., Headache, Dizziness, Drowsiness, Incoordination., slurred speech, slowed reaction time, giddiness, Unconsciousness  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

Headache  
Unconsciousness  
Cardiac irregularities  
narcosis

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 0.87 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 0.56 - 1 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 1 - 1.8 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test NOEC - Sewage sludge - 2 mg/l - 28 d (OECD Test Guideline 301D)

### 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d  
Result: > 91 - < 96 % - Readily biodegradable.  
(OECD Test Guideline 301C)

### 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. 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)

UN number: 3295 Class: 3 Packing group: II

Proper shipping name: Hydrocarbons, liquid, n.o.s.

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

#### IMDG

UN number: 3295 Class: 3 Packing group: II EMS-No: F-E, S-D

Proper shipping name: HYDROCARBONS, LIQUID, N.O.S. (Oct-1-ene)

Marine pollutant : yes

#### IATA

UN number: 3295 Class: 3 Packing group: II

Proper shipping name: Hydrocarbons, liquid, n.o.s. (Oct-1-ene)

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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.

#### Massachusetts Right To Know Components

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

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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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