

# • SAFETY DATA SHEET

Version 6.8  
Revision Date 11/06/2025  
Print Date 11/07/2025

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 4-Octyne

Product Number : 244473  
Brand : Aldrich  
CAS-No. : 1942-45-6

### 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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Flammable liquids : Category 3

Eye irritation : Category 2A

Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

Aspiration hazard : Category 1

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H226 Flammable liquid and vapour.  
H304 May be fatal if swallowed and enters airways.  
H319 Causes serious eye irritation.  
H335 May cause respiratory irritation.

Precautionary statements : **Prevention:**  
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.  
P261 Avoid breathing mist or vapours.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear protective gloves/ eye protection/ face protection.

**Response:**  
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.  
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.  
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P331 Do NOT induce vomiting.  
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.

**Storage:**

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.  
P405 Store locked up.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance  
CAS-No. : 1942-45-6

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4-Octyne	1942-45-6*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.  
Actual concentration is withheld as a trade secret

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### SECTION 4. FIRST AID MEASURES

General advice : Show this 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.

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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
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Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
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Specific hazards during fire fighting	: Combustible liquid.
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Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

Hazardous combustion products	: Carbon oxides
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Specific extinguishing methods	: No data available
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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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Special protective equipment for fire-fighters : In the event of fire, wear self-contained breathing apparatus.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Do not breathe vapours, 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.  
Advice for emergency responders:  
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.  
Risk of explosion.

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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.  
Take precautionary measures against static discharge.

Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.  
Keep away from heat and sources of ignition.

Storage class : 3, Flammable liquids

Recommended storage temperature : Recommended storage temperature see product label.

Packaging material : Suitable material: Mild Steel Drum

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

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.

Recommended Filter type: : Filter type ABEK

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.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Change contaminated clothing. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : colourless

Odor : characteristic

Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: -153 °F / -103 °C Method: lit.
Boiling point/boiling range	: 268 - 270 °F / 131 - 132 °C Method: lit.
Flash point	: 84 °F / 29 °C  Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: 37 %(V)
Lower explosion limit / Lower flammability limit	: 0.8 %(V)
Vapor pressure	: 12.9 hPa (77 °F / 25 °C)
Relative vapour density	: 1.4 (77 °F / 25 °C)
Relative density	: No data available
Density	: 0.751 g/cm <sup>3</sup> (77 °F / 25 °C) Method: lit.
Solubility(ies)	
Water solubility	: insoluble (68 °F / 20 °C)
Partition coefficient: n- octanol/water	: log Pow: 3.55 Method: (calculated) (Lit.) Bioaccumulation is not expected.
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available

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Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Refractive index	: 1.425 (68 °F / 20 °C) 589 nm
Molecular weight	: 110.20 g/mol
Particle characteristics	
Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapour/air-mixtures are explosive at intense warming.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Heating.
Incompatible materials	: Oxidizing agents
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

Inhalation: Irritating to respiratory system.

Dermal: 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

No data available

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### **Carcinogenicity**

- IARC: No component 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 component 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**

Inhalation - May cause respiratory irritation.

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

## **11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

No data available

### **Persistence and degradability**

No data available

### **Bioaccumulative potential**

#### **Components:**

#### **4-Octyne:**

Partition coefficient: n-octanol/water : log Pow: 3.55  
Method: (calculated)  
Remarks: (Lit.)  
Bioaccumulation is not expected.

### **Mobility in soil**

No data available

## Other adverse effects

### Components:

#### 4-Octyne:

Additional ecological information : We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Discharge into the environment must be avoided.

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : 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

### International Regulations

#### IATA-DGR

UN/ID No. : UN 3295  
Proper shipping name : Hydrocarbons, liquid, n.o.s.  
Class : 3  
Packing group : III  
Labels : Class 3 - Flammable liquids  
Packing instruction (cargo aircraft) : 366  
Packing instruction (passenger aircraft) : 355

#### IMDG-Code

UN number : UN 3295  
Proper shipping name : HYDROCARBONS, LIQUID, N.O.S.  
  
Class : 3  
Packing group : III  
Labels : 3  
EmS Code : F-E, S-D  
Marine pollutant : no

### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National Regulations

#### 49 CFR Road

UN/ID/NA number : UN 3295

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Proper shipping name : Hydrocarbons, liquid, n.o.s.  
Class : 3  
Packing group : III  
Labels : Class 3 - Flammable liquids  
ERG Code : 128  
Marine pollutant : no

Poison Inhalation Hazard : No

### **Special precautions for user**

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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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 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.

#### **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 components 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

### Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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Revision Date : 11/06/2025

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