

## SAFETY DATA SHEET

Version 6.0  
Revision Date 10/24/2019  
Print Date 06/01/2022

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

Product name : 2-Octynal

Product Number : 273643  
Brand : Aldrich  
CAS-No. : 1846-68-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

**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****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 4), H227  
Skin sensitisation (Category 1), H317  
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

Warning

|                            |                                                                                      |
|----------------------------|--------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                      |
| H227                       | Combustible liquid.                                                                  |
| H317                       | May cause an allergic skin reaction.                                                 |
| 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.                     |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.                               |
| P272                       | Contaminated work clothing must not be allowed out of the workplace.                 |
| P273                       | Avoid release to the environment.                                                    |
| P280                       | Wear protective gloves/ eye protection/ face protection.                             |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                      |
| P333 + P313                | If skin irritation or rash occurs: Get medical advice/ attention.                    |
| P363                       | Wash contaminated clothing before reuse.                                             |
| 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

|                  |                                    |
|------------------|------------------------------------|
| Formula          | : C <sub>8</sub> H <sub>12</sub> O |
| Molecular weight | : 124.18 g/mol                     |
| CAS-No.          | : 1846-68-0                        |
| EC-No.           | : 217-427-5                        |

| Component         | Classification                                                                                                         | Concentration |
|-------------------|------------------------------------------------------------------------------------------------------------------------|---------------|
| <b>Oct-2-ynal</b> |                                                                                                                        |               |
|                   | Flam. Liq. 4; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H227, H317, H400, H410<br>M-Factor - Aquatic Acute: 10 | <= 100 %      |

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

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Flush eyes with water as a precaution.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Unsuitable extinguishing media**

Do NOT use water jet.

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

Carbon oxides

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

## 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

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

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

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Air sensitive.

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

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and

components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### **Control of environmental exposure**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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

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

|                                                 |                                          |
|-------------------------------------------------|------------------------------------------|
| a) Appearance                                   | Form: liquid                             |
| b) Odour                                        | No data available                        |
| c) Odour Threshold                              | No data available                        |
| d) pH                                           | No data available                        |
| e) Melting point/freezing point                 | No data available                        |
| f) Initial boiling point and boiling range      | 74 - 76 °C 165 - 169 °F at 20 hPa - lit. |
| g) Flash point                                  | 68 °C (154 °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) Vapour pressure                              | No data available                        |
| l) Vapour density                               | No data available                        |
| m) Relative density                             | 0.871 g/mL at 25 °C (77 °F)              |
| n) Water solubility                             | No data available                        |
| o) Partition coefficient: n-octanol/water       | log Pow: 2.417                           |
| p) Auto-ignition temperature                    | No data available                        |
| 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**

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong oxidizing agents, Strong bases

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### 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

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

**Additional Information**

RTECS: Not available

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**

No data available

**12.2 Persistence and degradability**

No data available

**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 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life.

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**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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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. (Oct-2-ynal)

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.  
(Oct-2-ynal)  
Marine pollutant : yes

#### **IATA**

UN number: 3082    Class: 9    Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Oct-2-ynal)

#### **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**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### **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.

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

#### **Pennsylvania Right To Know Components**

|            |                      |               |
|------------|----------------------|---------------|
| Oct-2-ynal | CAS-No.<br>1846-68-0 | Revision Date |
|------------|----------------------|---------------|

|            |                      |               |
|------------|----------------------|---------------|
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#### **New Jersey Right To Know Components**

|            |                      |               |
|------------|----------------------|---------------|
| Oct-2-ynal | CAS-No.<br>1846-68-0 | Revision Date |
|------------|----------------------|---------------|



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## SECTION 16: Other information

### Further information

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