

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.1

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

### 1.1 Product identifiers

Product name : Methyl 2-octynoate

Product Number : 277509

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 111-12-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008

Skin sensitization (Sub-category 1A), H317

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 Label elements

### Labelling according Regulation (EC) No 1272/2008

#### Pictogram

|                                |                                                                        |
|--------------------------------|------------------------------------------------------------------------|
| Signal Word                    | Warning                                                                |
| Hazard statement(s)            |                                                                        |
| H317                           | May cause an allergic skin reaction.                                   |
| H410                           | Very toxic to aquatic life with long lasting effects.                  |
| Precautionary statement(s)     |                                                                        |
| P261                           | Avoid breathing mist or vapors.                                        |
| P272                           | Contaminated work clothing should not be allowed out of the workplace. |
| P273                           | Avoid release to the environment.                                      |
| P280                           | Wear protective gloves.                                                |
| P302 + P352                    | IF ON SKIN: Wash with plenty of water.                                 |
| P333 + P313                    | If skin irritation or rash occurs: Get medical advice/ attention.      |
| Supplemental Hazard Statements | none                                                                   |

### Reduced Labeling (<= 125 ml)

#### Pictogram

|                                |                                                                        |
|--------------------------------|------------------------------------------------------------------------|
| Signal Word                    | Warning                                                                |
| Hazard statement(s)            |                                                                        |
| H317                           | May cause an allergic skin reaction.                                   |
| Precautionary statement(s)     |                                                                        |
| P261                           | Avoid breathing mist or vapors.                                        |
| P272                           | Contaminated work clothing should not be allowed out of the workplace. |
| P280                           | Wear protective gloves.                                                |
| P302 + P352                    | IF ON SKIN: Wash with plenty of water.                                 |
| P333 + P313                    | If skin irritation or rash occurs: Get medical advice/ attention.      |
| Supplemental Hazard Statements | none                                                                   |

## 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

#### Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Formula : C<sub>9</sub>H<sub>14</sub>O<sub>2</sub>  
Molecular weight : 154,21 g/mol  
CAS-No. : 111-12-6  
EC-No. : 203-836-6

| Component                  |           | Classification                                                                                     | Concentration |
|----------------------------|-----------|----------------------------------------------------------------------------------------------------|---------------|
| <b>Methyl oct-2-ynoate</b> |           |                                                                                                    |               |
| CAS-No.                    | 111-12-6  | Skin Sens. 1A; Aquatic Acute 1; Aquatic Chronic 3; H317, H400, H412<br>M-Factor - Aquatic Acute: 1 | <= 100 %      |
| EC-No.                     | 203-836-6 |                                                                                                    |               |

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

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. Consult a physician.

##### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

##### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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**

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**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### **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. Chemisorb® ).

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**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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

### 8.2 Exposure controls

#### 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

required

##### Body Protection

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.

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.

##### 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) Physical state               | clear, liquid                                                                 |
| b) Color                        | light yellow                                                                  |
| c) Odor                         | No data available                                                             |
| d) Melting point/freezing point | Melting point/freezing point: < -50 °C at 1.013 hPa - OECD Test Guideline 102 |

- |                                                 |                                                                                     |
|-------------------------------------------------|-------------------------------------------------------------------------------------|
| e) Initial boiling point and boiling range      | 217 - 220 °C - lit.                                                                 |
| f) Flammability (solid, gas)                    | No data available                                                                   |
| g) Upper/lower flammability or explosive limits | No data available                                                                   |
| h) Flash point                                  | 89 °C - closed cup                                                                  |
| i) Autoignition temperature                     | 280 °C<br>at 1.013 hPa                                                              |
| j) Decomposition temperature                    | No data available                                                                   |
| k) pH                                           | No data available                                                                   |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available    |
| m) Water solubility                             | 0,151 g/l at 20 °C - OECD Test Guideline 105                                        |
| n) Partition coefficient: n-octanol/water       | log Pow: 3 at 20 °C - OECD Test Guideline 107 -<br>Bioaccumulation is not expected. |
| o) Vapor pressure                               | 0,1 hPa at 20 °C - OECD Test Guideline 104                                          |
| p) Density                                      | 0,92 g/cm <sup>3</sup> at 25 °C - lit.                                              |
| Relative density                                | No data available                                                                   |
| q) Relative vapor density                       | No data available                                                                   |
| r) Particle characteristics                     | No data available                                                                   |
|                                                 |                                                                                     |
| s) Explosive properties                         | No data available                                                                   |
| t) Oxidizing properties                         | none                                                                                |

## 9.2 Other safety information

|                 |                                                 |
|-----------------|-------------------------------------------------|
| Surface tension | 53,2 mN/m at 20 °C<br>- OECD Test Guideline 115 |
|-----------------|-------------------------------------------------|

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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:

Strong oxidizing agents  
Strong bases

#### **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 - Mouse - male and female - > 5.000 - < 10.000 mg/kg

Remarks: (ECHA)

Inhalation: No data available

Dermal: No data available

##### **Skin corrosion/irritation**

Skin - Guinea pig

Result: Mild skin irritation - 24 h

Remarks: (ECHA)

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

Eyes - Bovine cornea

Result: No eye irritation - 10 min

(OECD Test Guideline 437)

##### **Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

##### **Germ cell mutagenicity**

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

##### **Carcinogenicity**

No data available

##### **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****Endocrine disrupting properties****Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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**

|                                                     |                                                                                                                   |
|-----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| Toxicity to daphnia and other aquatic invertebrates | semi-static test EC50 - Daphnia magna (Water flea) - 0,62 mg/l - 48 h<br>(OECD Test Guideline 202)                |
| Toxicity to algae                                   | static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0,79 mg/l - 72 h<br>(OECD Test Guideline 201) |

**12.2 Persistence and degradability**

|                  |                                                                                                     |
|------------------|-----------------------------------------------------------------------------------------------------|
| Biodegradability | aerobic - Exposure time 28 d<br>Result: 80 % - Readily biodegradable.<br>(OECD Test Guideline 301F) |
|------------------|-----------------------------------------------------------------------------------------------------|

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**12.6 Endocrine disrupting properties****Product:**

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

**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

### 14.1 UN number

ADR/RID: 3082

IMDG: 3082

IATA: 3082

### 14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Methyl oct-2-ynoate)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Methyl oct-2-ynoate)

IATA: Environmentally hazardous substance, liquid, n.o.s. (Methyl oct-2-ynoate)

### 14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA: 9

### 14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

### 14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: yes

### 14.6 Special precautions for user

Tunnel restriction code : (-)

#### 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

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. E1 ENVIRONMENTAL HAZARDS

### Other regulations

Take note of Dir 94/33/EC on the protection of young people at work.

### 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

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## SECTION 16: Other information

### Full text of H-Statements referred to under sections 2 and 3.

|      |                                                       |
|------|-------------------------------------------------------|
| H317 | May cause an allergic skin reaction.                  |
| H400 | Very toxic to aquatic life.                           |
| H410 | Very toxic to aquatic life with long lasting effects. |
| H412 | May cause an allergic skin reaction.                  |

### Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

**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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