

## Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)  
Classifications according to Regulation (EC) No 1272/2008.  
Printdate 19 Mar 2025

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product name:

2-Octynoic acid methyl ester

### 1.1. Catalog No.:

692280

### 1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical  
uses: R&D

### 1.3. Uses advised against:

HPC Standards GmbH  
Am Wieseneck 7

04451 Cunnersdorf  
Deutschland

Tel. +49 34291 3372-36  
Fax. +49 34291 3372-39  
contact@hpc-standards.com

### 1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36  
This number is only available during office hours.

## 2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture  
Classification according to Regulation (EC) No 1272/2008  
Acute toxicity, Oral (Category 4), H302  
Skin irritation (Category 2), H315 Classification according to EU Directives 67/548/EEC or 1999/45/EC  
Xn Harmful R22, R38

### 2.2. Label elements

#### 2.2.1. Pictogram



#### 2.2.2.

2.2 Label elements  
Labelling according Regulation (EC) No 1272/2008  
Pictogram Signal word Warning  
Hazard statement(s)

H302 Harmful if swallowed.  
H315 Causes skin Irritation Precautionary statement(s) none  
Supplemental Hazard  
Statements  
none  
2.3 Other hazards - none

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances  
Synonyms : Methyl heptine carbonate  
NSC 72098  
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  
Hazardous ingredients according to Regulation (EC) No 1272/2008  
Component Classification Concentration  
Methyl oct-2-ynoate  
CAS-No.  
EC-No.  
111-12-6  
203-836-6  
Acute Tox. 4; Skin Irrit. 2;  
H302, H315  
≤ 100 %  
Hazardous ingredients according to Directive 1999/45/EC  
Component Classification Concentration  
Methyl oct-2-ynoate  
CAS-No.  
EC-No.  
111-12-6  
203-836-6  
Xn, R22 - R38 ≤ 100 %

#### 3.1.1. Formula

C<sub>9</sub>H<sub>14</sub>O<sub>2</sub>

#### 3.1.2. Molecular Weight (g/mol)

154.21

### 3.1.3. CAS-No.

111-12-6

## 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.

#### 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

## 5. FIRE-FIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

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

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

Carbon oxides

### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers

## 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. 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.

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13

## 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

Store in cool place. 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.

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

Components with workplace control parameters

### 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.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid

Colour: colourless

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

215 - 217 °C at 1.013 hPa

g) Flash point 89 °C - 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 0,920 g/cm<sup>3</sup> at 25 °C
  - n) Water solubility no data available
  - o) Partition coefficient: noctanol/  
water  
no data available
  - 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

## 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  
Other decomposition products - no data available
- In the event of fire: see section 5

## 11. TOXICOLOGICAL INFORMATION

- 11.1 Information on toxicological effects
- Acute toxicity
- LD50 Oral - rat - 1.530 mg/kg
- LD50 Dermal - rabbit - 3.300 mg/kg
- Skin corrosion/irritation
- Skin - rabbit
- Result: Skin irritation - 24 h
- 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.
- 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

Additional Information

RTECS: RI2735000

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

## 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

no data available

## 13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

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

Contaminated packaging

Dispose of as unused product

## 14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: - IMDG: - IATA: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

14.4 Packaging group

ADR/RID: - IMDG: - IATA: -

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for user

no data available

## 15. REGULATORY INFORMATION

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

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture  
no data available

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

## 16. OTHER 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. For lab use only!