

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Revision Date 07.07.2017

Version 1.5

**SECTION 1. Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Catalogue No. 814927

Product name Methyl octanoate for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 111-11-5

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

Identified uses Chemical for synthesis  
For additional information on uses please refer to the Merck Chemicals portal ([www.merckgroup.com](http://www.merckgroup.com)).

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

Company Merck KGaA \* 64271 Darmstadt \* Germany \* Phone:+49 6151 72-0

Responsible Department LS-QHC \* e-mail: [prodsafe@merckgroup.com](mailto:prodsafe@merckgroup.com)

**1.4 Emergency telephone number** Please contact the regional company representation in your country.

**SECTION 2. Hazards identification****2.1 Classification of the substance or mixture**

Classification (REGULATION (EC) No 1272/2008)

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Skin irritation, Category 2, H315

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

## 2.2 Label elements

**Labelling (REGULATION (EC) No 1272/2008)**

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*

H315 Causes skin irritation.

*Precautionary statements*

Prevention

P262 Do not get in eyes, on skin, or on clothing.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

**Reduced labelling ( $\leq 125$  ml)**

*Hazard pictograms*



*Signal word*

Warning

*CAS-No.* 111-11-5

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula  $C_9H_{18}O_2$  (Hill)  
EC-No. 203-835-0  
Molar mass 158,24 g/mol

#### Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical name (Concentration)*

CAS-No.	Registration number	Classification
methyl octanoate ( $\leq 100\%$ )		
111-11-5	*)	

Skin irritation, Category 2, H315

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

### 3.2 Mixture

Not applicable

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower.

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

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

### 4.2 Most important symptoms and effects, both acute and delayed

The Safety Data Sheets for catalogue items are available at [www.merckgroup.com](http://www.merckgroup.com)

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irritant effects

#### 4.3 Indication of any immediate medical attention and special treatment needed

No information 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

Combustible.

Vapours 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

*Special protective equipment 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.

*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 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:

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Protective equipment 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. Chemizorb®). Dispose of properly. Clean up affected area.

## 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

#### *Advice on safe handling*

Observe label precautions.

#### *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.

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

#### *Storage conditions*

Tightly closed.

Recommended storage temperature see product label.

### 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

### 8.2 Exposure controls

#### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

#### Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

#### *Eye/face protection*

Safety glasses

#### *Hand protection*

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 730 Camatril® -Velours (full contact), KCL 898 Butoject® (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

### *Other protective equipment*

Flame retardant antistatic protective clothing.

### *Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

### **Environmental exposure controls**

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**

Form	liquid
Colour	colourless
Odour	ester-like
Odour Threshold	No information available.
pH	No information available.
Melting point	-40 °C
Boiling point/boiling range	193 °C at 1.013 hPa

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Flash point	ca. 68 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	1,33 hPa at 34,2 °C
Relative vapour density	No information available.
Density	0,877 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	0,064 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,3 (calculated) (IUCALID) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.



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Oxidizing properties none

## 9.2 Other data

none

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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 acids, strong alkalis, strong reducing agents

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

no information available

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

*Acute oral toxicity*

LD50 Rat: > 2.000 mg/kg

(IUCLID)

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## *Acute inhalation toxicity*

This information is not available.

## *Acute dermal toxicity*

This information is not available.

## *Skin irritation*

Irritating to skin.

Causes skin irritation.

## *Eye irritation*

slight irritation

## *Sensitisation*

This information is not available.

## *Germ cell mutagenicity*

This information is not available.

## *Carcinogenicity*

This information is not available.

## *Reproductive toxicity*

This information is not available.

## *Teratogenicity*

This information is not available.

## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Aspiration hazard*

This information is not available.

## 11.2 Further information

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

LC50 *Leuciscus idus* (Golden orfe): 95 mg/l; 48 h

DIN 38412 part 15

(above the solubility limit in the test medium)

### 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 3,3

(calculated)

(IUCLID) Bioaccumulation is not expected.

### 12.4 Mobility in soil

No information 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

*Additional ecological information*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

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

### Land transport (ADR/RID)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

### Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

### 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard SEVESO III

Legislation Not applicable

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

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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1\%$  (w/w).

#### *National legislation*

Storage class 10

## 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.

H315 Causes skin irritation.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

#### *Hazard pictograms*



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## *Signal word*

Warning

## *Hazard statements*

H227 Combustible liquid.

H315 Causes skin irritation.

## *Precautionary statements*

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P313 Get medical advice/ attention.

## **Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

## **Regional representation**

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*