



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 14.08.2015

Version 3.5

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

### 1.1 Product identifier

Catalogue No.	800202
Product name	Ethyl 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.	106-32-1

### 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 ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).
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### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	EQ-RS * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

### 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

This substance is not classified as dangerous according to European Union legislation.

### 2.2 Label elements

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

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

### 2.3 Other hazards

None known.

## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	$\text{CH}_3(\text{CH}_2)_6\text{COOC}_2\text{H}_5$	$\text{C}_{10}\text{H}_{20}\text{O}_2$ (Hill)
EC-No.	203-385-5	
Molar mass	172,27 g/mol	
Remarks	No disclosure requirement according to Regulation (EC) No. 1907/2006.	

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**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.

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**

We have no description of any toxic symptoms.

**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*

Carbon dioxide (CO<sub>2</sub>), Foam, 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*

In the event of fire, wear self-contained breathing apparatus.

*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. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

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**

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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*

Change contaminated clothing. Wash hands 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

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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.

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).

*Other protective equipment*

Flame retardant antistatic protective clothing.

*Respiratory protection*

Not required; except in case of aerosol formation.

**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	characteristic
Odour Threshold	No information available.
pH	No information available.
Melting point	-47 °C
Boiling point/boiling range	208 °C at 1.013 hPa
Flash point	79 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	0,7 %(V)
Upper explosion limit	No information available.
Vapour pressure	0,2 hPa at 20 °C  3,18 hPa at 60 °C

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Relative vapour density	5,93
Density	0,87 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	0,070 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 3,81 (calculated) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	> 300 °C
Viscosity, dynamic	< 30 mPa.s
Explosive properties	Not classified as explosive.
Oxidizing properties	none

**9.2 Other data**

Ignition temperature 325 °C

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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:  
Oxidizing agents, Bases, Reducing agents, acids

**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: 25.960 mg/kg

(RTECS)

*Acute inhalation toxicity*

This information is not available.

*Acute dermal toxicity*

LD50 Rabbit: > 5.000 mg/kg

(External MSDS)

*Skin irritation*

Rabbit

Result: slight irritation

(External MSDS)

*Eye irritation*

This information is not available.

*Sensitisation*

Patch test: human

Result: negative

(External MSDS)

*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**

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**

**12.1 Toxicity**

No information available.

**12.2 Persistence and degradability**

No information available.

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**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*  
log Pow: 3,81  
(calculated)

(Lit.) 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**

*Henry constant*  
128,65 Pa\*m<sup>3</sup>/mol  
(calculated) (Lit.) Distribution preferentially in air.

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

*National legislation*

Storage class 10

**15.2 Chemical Safety Assessment**

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For this product a chemical safety assessment was not carried out.

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**SECTION 16. Other information**

**Training advice**

Provide adequate information, instruction and training for operators.

**Labelling**

*Signal word*

Warning

*Hazard statements*

H227 Combustible liquid.

**Labelling (67/548/EEC or 1999/45/EC)**

The product does not need to be labelled in accordance with EC directives or respective national laws.

**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.*