



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 05.11.2010

Version 5.5

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

### 1.1 Product identifier

Catalogue No.	800190
Product name	Ethyl hexanoate 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.

### 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.merck-chemicals.com">www.merck-chemicals.com</a> ).
-----------------	---

### 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.
--------------------------------	---

## 2. Hazards identification

### 2.1 Classification of the substance or mixture

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

Flammable liquid, Category 3, H226

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

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

R10

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 2.2 Label elements

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

*Hazard pictograms*



*Signal word*

Warning

*Hazard statements*

H226 Flammable liquid and vapour.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

*Precautionary statements*  
P210 Keep away from heat.

Reduced labelling (≤125 ml)

*Hazard pictograms*



*Signal word*  
Warning

CAS-No. 123-66-0

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

R-phrase(s) 10 Flammable.  
EC-No. 204-640-3

**2.3 Other hazards**

None known.

---

**3. Composition/information on ingredients**

Formula	$\text{CH}_3(\text{CH}_2)_4\text{COOC}_2\text{H}_5$	$\text{C}_8\text{H}_{16}\text{O}_2$ (Hill)
CAS-No.	123-66-0	
EC-No.	204-640-3	
Molar mass	144,21 g/mol	

---

**4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

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**

irritant effects, Cough, Shortness of breath, respiratory arrest, Dermatitis, Dizziness,  
Unconsciousness, inebriation, drowsiness  
Drying-out effect resulting in rough and chapped skin.

**4.3 Indication of immediate medical attention and special treatment needed**

No information available.

---

**5. Fire-fighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

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

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

*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 material, Vapours are heavier than air and may spread along floors.  
Forms explosive mixtures with air at elevated temperatures.  
Development of hazardous combustion gases or vapours possible in the event of fire.

**5.3 Advice for firefighters**

*Special protective equipment for fire-fighters*

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

*Further information*

Cool closed containers exposed to fire with water spray. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

**6. Accidental release measures**

**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Ensure adequate ventilation. 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 empty into drains. Risk of explosion.

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

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7.2 and 10.5).

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.

---

**7. Handling and storage**

**7.1 Precautions for 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.

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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store at +15°C to +25°C.

**7.3 Specific end uses**

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

---

**8. Exposure controls/personal protection**

**8.1 Control parameters**

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

## 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.

#### *Hygiene measures*

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

#### *Eye/face protection*

Safety glasses

#### *Hand protection*

splash contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 60 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 890 Vitoject® (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](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 empty into drains.

Risk of explosion.

---

## 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

Odour	like fruit
Odour Threshold	No information available.
pH	No information available.
Melting point	-67 °C
Boiling point/boiling range	166 °C
Flash point	52 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	0,9 %(V)
Upper explosion limit	No information available.
Vapour pressure	< 1,33 hPa at 25 °C
Relative vapour density	4,98
Relative density	0,87 g/cm <sup>3</sup> at 20 °C
Water solubility	0,63 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 2,83 Method: (calculated) (Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Oxidizing properties	No information available.

## 9.2 Other data

Ignition temperature 395 °C

---

## 10. Stability and reactivity

### 10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

**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

**10.4 Conditions to avoid**

Heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**10.5 Incompatible materials**

various plastics

**10.6 Hazardous decomposition products**

no information available

---

**11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 rat

Dose: > 5.000 mg/kg

(External MSDS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

*Acute inhalation toxicity*

Symptoms: mucosal irritations, Cough, Shortness of breath

*Acute dermal toxicity*

LD50 rabbit

Dose: > 5.000 mg/kg

(External MSDS)

*Skin irritation*

rabbit

Result: slight irritation

(RTECS) Drying-out effect resulting in rough and chapped skin. Dermatitis

*Eye irritation*

slight irritation

*Genotoxicity in vitro*

Ames test

Result: negative

(Lit.)

*Specific target organ toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*

No aspiration toxicity classification

**11.2 Further information**

*Further information*

After absorption:

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

Systemic effects:

drowsiness, Dizziness, inebriation, Unconsciousness, respiratory arrest

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

---

## 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

LC50

Species: Pimephales promelas (fathead minnow)

Dose: 8,9 mg/l

Exposure time: 96 h

(ECOTOX Database)

### 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 2,83

Method: (calculated)

(Lit.) No remarkable bioaccumulation potential is expected (log Pow 1-3).

### 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*

Do not allow to run into surface waters, wastewater, or soil.

---

## 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.

---

## 14. Transport information

### ADR/RID

UN 1993 FLAMMABLE LIQUID, N.O.S. (ETHYLHEXANOATE), 3, III

### IATA

UN 1993 FLAMMABLE LIQUID, N.O.S. (ETHYLHEXANOATE), 3, III

### IMDG

UN 1993 FLAMMABLE LIQUID, N.O.S. (ETHYLHEXANOATE), 3, III

EmS

F-E S-E

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

---

## 15. Regulatory information

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

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

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 800190  
Product name Ethyl hexanoate for synthesis

---

*EU regulations*

Major Accident Hazard 96/82/EC  
Legislation Flammable.  
6  
Quantity 1: 5.000 t  
Quantity 2: 50.000 t

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

*National legislation*

Storage class VCI 3 Flammable Liquids

### 15.2 Chemical Safety Assessment

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

---

### 16. Other information

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

H226 Flammable liquid and vapour.

**Full text of R-phrases referred to under sections 2 and 3**

R10 Flammable.

**Training advice**

Provide adequate information, instruction and training for operators.

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

**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).

---

*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.*