

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 16.05.2011

Version 5.0

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

1.1 Product identifier

Catalogue No.	814926
Product name	Methyl heptanoate 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 (www.merck-chemicals.com).
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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	LS-QHC * e-mail: prodsafe@merckgroup.com

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H226 Flammable liquid and vapour.

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

CAS-No. 106-73-0

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.

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	C ₈ H ₁₆ O ₂ (Hill)
CAS-No.	106-73-0
EC-No.	203-428-8
Molar mass	144,21 g/mol

SECTION 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 with the eyelid held wide open. Call in ophthalmologist if necessary.

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, Drying-out effect resulting in rough and chapped skin.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), 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 material, Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

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

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Cool closed containers exposed to fire with water spray.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. 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 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.

SECTION 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.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

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. Wash hands after working with substance.

Eye/face protection

Safety glasses

Hand protection

splash contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 120 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 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

required when vapours/aerosols are generated.

Environmental exposure controls

Do not empty into drains.
Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	like fruit
Odour Threshold	No information available.
pH	No information available.
Melting point	-56 °C

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

Boiling point/boiling range	173 °C at 1.013 hPa
Flash point	57 °C
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Relative density	0,880 g/cm ³ at 20 °C
Water solubility	at 20 °C insoluble
Partition coefficient: n-octanol/water	log Pow: 2,83 (calculated) (Lit.) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	< 30 mPa.s
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

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 bases, 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.

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 rat: > 5.000 mg/kg (RTECS)

Acute dermal toxicity

LD50 rabbit: > 5.000 mg/kg (RTECS)

Skin irritation

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Sensitisation

Sensitization possible in predisposed persons.

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

Based on available data the classification criteria are not met.

11.2 Further information

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,83

(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

Additional ecological information

We have no quantitative data concerning the ecological effects of this product.

Biological effects:

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

Catalogue No. 814926
Product name Methyl heptanoate for synthesis

When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected.

Further information on ecology

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

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

ADR/RID

UN 3272 ESTERS, N.O.S. (METHYL HEPTANOATE), 3, III

IATA

UN 3272 ESTERS, N.O.S. (METHYL HEPTANOATE), 3, III

IMDG

UN 3272 ESTERS, N.O.S. (METHYL HEPTANOATE), 3, III

EmS F-E S-D

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.

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC

Legislation Directive 96/82/EC does not apply

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

|| Storage class 3

15.2 Chemical Safety Assessment

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

SECTION 16. Other information

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

H226 Flammable liquid and vapour.

Training advice

Provide adequate information, instruction and training for operators.

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.

Regional representation

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

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

Catalogue No.	814926
Product name	Methyl heptanoate for synthesis

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.