



SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Date of issue: 01.09.2013

Version 1.0

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

1.1 Product identifier

Catalogue No. 820624
Product name 1-Heptanol 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).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department EHS Manager *+61 (3) 8727 6300 * Monday through Friday, 8:00am to 5:00pm (EST)
Regional representation Merck Pty. Limited
ABN 80 001 239 818
Ground Floor, Building 1
885 Mountain Highway
Bayswater VIC 3153 Australia
www.merckmillipore.com

1.4 Emergency telephone number

+61 (3) 8727 6300
After hours: CHEMCALL +64 4 917 9888
Poisons Information Centre: 13 1126

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Dermal, H312
Acute toxicity, Category 4, Oral, H302
Eye irritation, Category 2, H319

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

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

Xn	Harmful	R21/22
Xi	Irritant	R36

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

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word
Warning

Hazard statements

H302 + H312 Harmful if swallowed or in contact with skin
H319 Causes serious eye irritation.

Precautionary statements

Response

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

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word
Warning

CAS-No. 111-70-6

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ (CH ₂) ₆ OH	C ₇ H ₁₆ O (Hill)
CAS-No.	111-70-6	
EC-No.	203-897-9	
Molar mass	116,2 g/mol	

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

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
Heptan-1-ol (<= 100 %)		
111-70-6	*	Acute toxicity, Category 4, H312 Acute toxicity, Category 4, H302 Eye irritation, Category 2, H319

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

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
Heptan-1-ol (<= 100 %)	
111-70-6	Xn, Harmful; R21/22 Xi, Irritant; R36

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

3.2 Preparation
not applicable

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. Get medical attention.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, narcosis, Diarrhoea, Nausea, Vomiting, Headache

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting 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 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.

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Further information

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

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. 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.

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. Chemisorb®). 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

Advice on safe handling

Observe label precautions.

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.

Store at +15°C to +25°C.

7.3 Specific end use(s)

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

Contains no substances with occupational exposure limit values.

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.

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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:	polychloroprene
Glove thickness:	0,65 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 730 Camatril® -Velours (full contact), KCL 720 Camapren® (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

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.

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	-35 °C

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Boiling point/boiling range	176 °C at 1.013 hPa
Flash point	78 °C Method: c.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	0,5 hPa at 20 °C
Relative vapour density	4,01
Relative density	0,82 g/cm ³ at 20 °C
Water solubility	1 g/l at 18 °C
Partition coefficient: n-octanol/water	log Pow: 2,62 (experimental) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	7,4 mPa.s at 20 °C
Explosive properties	No information available.
Oxidizing properties	No information available.

9.2 Other data

Ignition temperature 350 °C

SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

increased reactivity with:

Strong acids, Oxidizing agents

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10.4 Conditions to avoid

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

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: 500 mg/kg (RTECS)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

absorption

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 rabbit: 2.000 mg/kg (RTECS)

absorption

Skin irritation

rabbit

Result: No irritation

(External MSDS)

Eye irritation

Causes serious eye irritation.

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vitro

Mutagenicity (mammal cell test): chromosome aberration.

Result: negative

(External MSDS)

Ames test

Result: negative

(External MSDS)

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.

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Aspiration hazard

This information is not available.

11.2 Further information

Systemic effects:

Nausea, Vomiting, Diarrhoea, narcosis, Headache

Other information

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 34,5 mg/l; 96 h (ECOTOX Database)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia pulex (Water flea): 49 mg/l; 48 h (ECOTOX Database)

EC50 Tetrahymen pyriformis: 112 mg/l; 48 h (ECOTOX Database)

Toxicity to bacteria

EC5 Pseudomonas putida: 67 mg/l; 16 h (External MSDS)

12.2 Persistence and degradability

Ratio BOD/ThBOD

BOD5 56,3 %

(HSDB)

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,62

(experimental)

Bioaccumulation is not expected. (Lit.)

12.4 Mobility in soil

Distribution among environmental compartments

log Koc: 1,92

Mobility of the substance in soil is expected (log koc <3). (External MSDS)

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

Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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

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

SECTION 15. Regulatory information

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

National legislation

Storage class 10 - 13

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.

H302 Harmful if swallowed.
H312 Harmful in contact with skin.
H319 Causes serious eye irritation.

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

R21/22 Harmful in contact with skin and if swallowed.
R36 Irritating to eyes.


Training advice

Provide adequate information, instruction and training for operators.


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

Symbol(s)  Xn Harmful
R-phrase(s) 21/22-36 Harmful in contact with skin and if swallowed. Irritating to eyes.
S-phrase(s) 36/37 Wear suitable protective clothing and gloves.
EC-No. 203-897-9

Reduced labelling (≤125 ml)

Symbol(s)  Xn Harmful
R-phrase(s) 21/22 Harmful in contact with skin and if swallowed.
S-phrase(s) 36/37 Wear suitable protective clothing and gloves.

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.

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.