

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 25.06.2014

Version 3.5

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

### 1.1 Product identifier

Catalogue No.	841753
Product name	1-Heptanethiol 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.	1639-09-4

### 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> ).
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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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

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.

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

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*Hazard statements*

H226 Flammable liquid and vapour.

*Precautionary statements*

Prevention

P210 Keep away from heat.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*

Warning

CAS-No. 1639-09-4

**2.3 Other hazards**

None known.

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**SECTION 3. Composition/information on ingredients**

**3.1 Substance**

Formula C<sub>7</sub>H<sub>16</sub>S (Hill)  
EC-No. 216-678-8  
Molar mass 132,26 g/mol

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

Remarks No disclosure requirement according to Regulation (EC) No. 1907/2006

**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**

Irritation and corrosion, Cough, Shortness of breath, Risk of blindness!

**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>), Dry powder, Foam

*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 at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

Sulphur oxides

Caution! in contact with water product releases:

hydrochloric acid

### 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. Suppress (knock down) gases/vapours/mists with a water spray jet. 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: Avoid substance contact. Do not breathe vapours, aerosols. 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: 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 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.

Keep workplace dry. Do not allow product to come into contact with water.

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*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*

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

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:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 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 898 Butoject® (full contact), KCL 730 Camatril® -Velours (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)).

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*Other protective equipment*

Flame retardant antistatic protective clothing

*Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: Filter B (acc. to DIN 3181) for inorganic gases and vapours

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.

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**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	liquid
Colour	colourless
Odour	malodorous
Odour Threshold	No information available.
pH	No information available.
Melting point	-43 °C
Boiling point/boiling range	173 - 175 °C at 1.013 hPa
Flash point	46 °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	1,5 hPa at 25 °C
Relative vapour density	No information available.
Density	0,844 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	0,009 g/l at 20 °C

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Partition coefficient: n-octanol/water log Pow: 3,72  
(calculated)  
(Lit.) 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.

Oxidizing properties none

## 9.2 Other data

none

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## 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:

Bases, Strong oxidizing agents, strong reducing agents, Alkali metals

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

This information is not available.

#### *Acute inhalation toxicity*

This information is not available.

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

This information is not available.

#### *Eye irritation*

This information is not available.

#### *Sensitisation*

This information is not available.

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*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**

The following applies to mercaptans in general: offensive odour.

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.

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 3,72

(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*

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 UN number UN 3071  
14.2 Proper shipping name MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (1-HEPTANETHIOL)  
14.3 Class 6.1 (3)  
14.4 Packing group II  
14.5 Environmentally hazardous --  
14.6 Special precautions for user yes  
Tunnel restriction code D/E

**Inland waterway transport (ADN)**

Not relevant

**Air transport (IATA)**

14.1 UN number UN 3071  
14.2 Proper shipping name MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (1-HEPTANETHIOL)  
14.3 Class 6.1 (3)  
14.4 Packing group II  
14.5 Environmentally hazardous --  
14.6 Special precautions for user no

**Sea transport (IMDG)**

14.1 UN number UN 3071  
14.2 Proper shipping name MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (1-HEPTANETHIOL)  
14.3 Class 6.1 (3)  
14.4 Packing group II  
14.5 Environmentally hazardous --  
14.6 Special precautions for user yes  
EmS F-E S-D

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*



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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.

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

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

Regulation (EC) No 689/2008 concerning the export not regulated  
and import of dangerous chemicals

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 3

## 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.

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.

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

*R-phrases* 10 Flammable.  
EC-No. 216-678-8

### 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.*