

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 17.11.2017

Version 6.5

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

1.1 Product identifier

Catalogue No. 814444

Product name 1-Octadecanethiol 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. 2885-00-9

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.merckgroup.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 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

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Precautionary statements

Prevention

P262 Do not get in eyes, on skin, or on clothing.

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	$\text{CH}_3-(\text{CH}_2)_{16}-\text{CH}_2-\text{SH}$	$\text{C}_{18}\text{H}_{38}\text{S}$ (Hill)
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EC-No.	220-744-1
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Molar mass	286,55 g/mol
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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. Remove contact lenses.

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, Dermatitis

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.

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.

Fire may cause evolution of:

Sulphur oxides

5.3 Advice for firefighters

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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

Suppress (knock down) gases/vapours/mists with a water spray jet. 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 inhalation of dusts. 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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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

Change contaminated clothing. Wash hands after working with substance.

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7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

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.

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:	0,11 mm
Break through time:	> 480 min

splash contact:

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Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 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 741 Dermatril® L (full contact), KCL 741 Dermatril® L (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 dusts are generated.

Recommended Filter type: Filter B-(P2)

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 let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	solid
Colour	white

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Odour	malodorous
Odour Threshold	No information available.
pH	No information available.
Melting point/range	28 - 31 °C
Boiling point/boiling range	366 °C
Flash point	185 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	< 0,5 hPa at 20 °C
Relative vapour density	No information available.
Density	0,847 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C insoluble

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Partition coefficient: n-octanol/water	log Pow: 9,12 (calculated) (Lit.) Potential bioaccumulation
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Auto-ignition temperature	No information available.
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Decomposition temperature	> 300 °C
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Viscosity, dynamic	No information available.
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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9.2 Other data

Ignition temperature	> 200 °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.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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:

Alkali metals, Oxidizing agents, Reducing agents, Strong acids, alkalines

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10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 5.000 mg/kg

(Lit.)

Symptoms: Irritation of mucous membranes

Acute inhalation toxicity

Symptoms: Irritations of mucous membranes

Acute dermal toxicity

LD50 Rat: > 2.000 mg/kg

(Lit.)

Skin irritation

Possible damages: Irritations Dermatitis

Eye irritation

Possible damages: Irritations

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.

However, when the product is handled appropriately, hazardous effects are unlikely to occur.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 fish: > 100 mg/l; 48 h

(External MSDS)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia (water flea): > 100 mg/l

(External MSDS)

12.2 Persistence and degradability

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Biodegradability

0 %; 28 d

OECD Test Guideline 301C

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 9,12

(calculated)

(Lit.) Potential bioaccumulation

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.

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

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)

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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

EU regulations

Major Accident Hazard	SEVESO III
Legislation	Not applicable

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

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

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 10 - 13

15.2 Chemical safety assessment

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

SECTION 16. Other information

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.

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.