



# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.04.2014

Version 2.0

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

### 1.1 Product identifier

Catalogue No.	804393
Product name	1-Hexanol 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.	111-27-3

### 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	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 <a href="http://www.merckmillipore.com">www.merckmillipore.com</a>

### 1.4 Emergency telephone number

+61 (3) 8727 6300  
After hours: CHEMCALL 1800 127 406  
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, Oral, H302  
Flammable liquid, Category 3, H226  
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	R22
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

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

#### Precautionary statements

##### Prevention

P210 Keep away from heat.

##### Response

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 ( $\leq 125$ ml)

##### Hazard pictograms



##### Signal word

Warning

CAS-No. 111-27-3

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula  $C_6H_{14}O$  (Hill)  
EC-No. 203-852-3  
Molar mass 102.18 g/mol

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

#### Chemical Name (Concentration)

CAS-No. Registration number Classification

hexan-1-ol ( $\leq 100\%$ )

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

111-27-3 \*)

Flammable liquid, Category 3, H226  
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
hexan-1-ol (<= 100 %)	
111-27-3	Xn, Harmful; R22 Xi, Irritant; R36

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

**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.

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

After eye contact: rinse out with plenty of water. 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, Cough, narcosis, Diarrhoea, Nausea, Vomiting, Headache

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

Laxative: Sodium sulfate (1 tablespoon/1/4 l water).

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**SECTION 5. Firefighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), 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 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 firefighters*

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.

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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.

**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.

*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. Preventive skin protection recommended. Wash hands after working with substance.

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

*Storage conditions*

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

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**

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:	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)).

*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.

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**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.

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Melting point	-45 °C Method: ASTM D 97-66
Boiling point/boiling range	155 °C at 1,015 hPa Method: ASTM D 1120-72
Flash point	60 °C at 1,015 hPa  Method: ASTM D 93
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1.2 %(V)
Upper explosion limit	7.7 %(V)
Vapour pressure	3.64 hPa at ca. 38 °C Method: ASTM D 2879-86  1 hPa at 20 °C
Relative vapour density	3.5
Density	0.82 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	5.9 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2.03 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0.592 mPa.s at 25 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

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Ignition temperature 285 °C  
Method: DIN 51794

Viscosity, kinematic 3.64 mm<sup>2</sup>/s  
at 40 °C  
Method: ASTM D 445

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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:

Strong oxidizing agents, halogens

Risk of ignition or formation of inflammable gases or vapours with:

Alkali metals, Alkaline earth metals, Aluminium

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

various plastics

### 10.6 Hazardous decomposition products

no information available

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 rat: 200 - 2,000 mg/kg

OECD Test Guideline 401

absorption

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

#### *Acute inhalation toxicity*

LC50 rat: > 21 mg/l; 1 h (ECHA)

Symptoms: Possible damages:, mucosal irritations, Cough

#### *Acute dermal toxicity*

LD50 rabbit: > 2,000 mg/kg

OECD Test Guideline 402

absorption

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*Skin irritation*

rabbit

Result: slight irritation

OECD Test Guideline 404

*Eye irritation*

rabbit

Result: irritating

OECD Test Guideline 405

Causes serious eye irritation.

*Sensitisation*

Sensitisation test (Magnusson and Kligman):

Result: negative

Method: OECD Test Guideline 406

*Germ cell mutagenicity*

*Genotoxicity in vivo*

Mutagenicity (mammal cell test): micronucleus.

mouse

Result: negative

Method: OECD Test Guideline 474

*Genotoxicity in vitro*

Ames test

Result: negative

Method: OECD Test Guideline 471

*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

Systemic effects:

After absorption of large quantities:

Nausea, Vomiting, Diarrhoea, Headache, narcosis

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

Limit Test LC50 Pimephales promelas (fathead minnow): 97 mg/l; 96 h

US-EPA

*Toxicity to daphnia and other aquatic invertebrates*

EC50 Tetrahymen pyriformis: 300 mg/l; 48 h (ECOTOX Database)

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EC50 Daphnia magna (Water flea): 201 mg/l; 24 h (ECHA)

*Toxicity to algae*

static test NOEC Pseudokirchneriella subcapitata (green algae): 11.3 mg/l; 72 h

OECD Test Guideline 201

*Toxicity to bacteria*

EC10 Pseudomonas putida: 3,000 mg/l; 30 min

DIN 38412 (IUCLID)

**12.2 Persistence and degradability**

*Biodegradability*

61.8 %; 30 d; aerobic

OECD Test Guideline 301D

Readily biodegradable.

*Ratio BOD/ThBOD*

BOD5 28 %

(Lit.)

*Ratio COD/ThBOD*

94 %

(Lit.)

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 2.03

(experimental)

(Lit.) Bioaccumulation is not expected.

**12.4 Mobility in soil**

No information available.

**12.5 Results of PBT and vPvB assessment**

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

**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](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 2282  
14.2 Proper shipping name HEXANOLS  
14.3 Class 3  
14.4 Packing group III  
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 2282  
14.2 Proper shipping name HEXANOLS  
14.3 Class 3  
14.4 Packing group III  
14.5 Environmentally hazardous --  
14.6 Special precautions for user no

**Sea transport (IMDG)**

14.1 UN number UN 2282  
14.2 Proper shipping name HEXANOLS  
14.3 Class 3  
14.4 Packing group III  
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

**Other regulations**

Hazchem Code 3Y

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**SECTION 15. Regulatory information**

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

*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.  
H302 Harmful if swallowed.  
H319 Causes serious eye irritation.


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

R22 Harmful if swallowed.  
R36 Irritating to eyes.

**Training advice**

Provide adequate information, instruction and training for operators.

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

*Symbol(s)*  Xn Harmful

*R-phrase(s)* 22-36 Harmful if swallowed. Irritating to eyes.

*S-phrase(s)* 24/25 Avoid contact with skin and eyes.

EC-No. 203-852-3

**Reduced labelling (≤125 ml)**

*Symbol(s)*  Xn Harmful

*R-phrase(s)* 22 Harmful if swallowed.

*S-phrase(s)* 24/25 Avoid contact with skin and eyes.

**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).

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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.*