

Safety Data Sheet

according to Regulation (EC) No 1907/2006

1-Hexanol > 98 % for synthesis

Revision date: 31.07.2023

Product code: 28020

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

1.1. Product identifier

1-Hexanol > 98 % for synthesis

REACH Registration Number: 01-2119487967-12-XXXX
CAS No: 111-27-3
Index No: 603-059-00-6
EC No: 203-852-3

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture

Laboratory chemicals

Industrial uses: Uses of substances as such or in preparations at industrial sites

Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit

Telefax: 0203/5194-290

Telephone: 0203/5194-107/117

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

No data available

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 3; H226
Acute Tox. 4; H312
Acute Tox. 4; H302
Eye Irrit. 2; H319

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning

Pictograms:



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Hazard statements

H226 Flammable liquid and vapour.
H302+H312 Harmful if swallowed or in contact with skin.
H319 Causes serious eye irritation.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
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.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C6H14O
Molecular weight: 102,18 g/mol

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
111-27-3	hexan-1-ol			100 %
	203-852-3	603-059-00-6	01-2119487967-12-XXXX	
	Flam. Liq. 3, Acute Tox. 4, Acute Tox. 4, Eye Irrit. 2; H226 H312 H302 H319			

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
	Specific Conc. Limits, M-factors and ATE		
111-27-3	203-852-3	hexan-1-ol	100 %
	dermal: LD50 = 1500 - 2000 mg/kg; oral: LD50 = 3210 mg/kg		

Further Information

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 = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.

After contact with skin

Wash immediately with: Water
Take off immediately all contaminated clothing and wash it before reuse.
Call a physician immediately.

After contact with eyes

Rinse immediately carefully and thoroughly with eye-bath or water.
Remove contact lenses, if present and easy to do. Continue rinsing.

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Consult an ophthalmologist.

After ingestion

Observe risk of aspiration if vomiting occurs.

Call a physician immediately.

4.2. Most important symptoms and effects, both acute and delayed

Cough

Narcotic effects

Gastrointestinal complaints

Headache

Irritant

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

Give sodium sulfate as laxative (1 tablespoon in 1 glass of water).

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Foam

Carbon dioxide (CO₂)

Extinguishing powder

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible liquids

Hazardous combustion products

In case of fire may be liberated:

Carbon dioxide (CO₂) Carbon monoxide

In case of warming:

Vapours are heavier than air, spread along floors and form explosive mixtures with air.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

In case of fire and/or explosion do not breathe fumes.

Avoid contact with skin, eyes and clothes.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

Move undamaged containers from immediate hazard area if it can be done safely.

Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Keep away from sources of ignition - No smoking.

This material can be ignited by heat, sparks, flames, or other sources of ignition (e.g., static electricity, pilot lights, mechanical/electrical equipment, and electronic devices such as cell phones, computers, calculators, and pagers which have not been certified as intrinsically safe).

Take action to prevent static discharges.

For non-emergency personnel

Provide adequate ventilation.

Use personal protection equipment.

Avoid contact with skin, eyes and clothes.

Remove persons to safety.

Emergency procedures

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Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

Danger of explosion

6.3. Methods and material for containment and cleaning up

For containment

Cover drains.

Prevent spread over a wide area (e.g. by containment or oil barriers).

Collect in closed and suitable containers for disposal.

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.

Do not breathe dust/fume/gas/mist/vapours/spray.

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Use personal protection equipment.

Do not breathe gas/fumes/vapour/spray.

Provide adequate ventilation.

Read label before use.

Advice on protection against fire and explosion

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Take precautionary measures against static discharges.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

Further information on handling

Take off immediately all contaminated clothing and wash it before reuse.

Wash hands before breaks and after work.

Draw up and observe skin protection programme.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed and dry.

Hints on joint storage

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Further information on storage conditions

Store in a well-ventilated place. Keep container tightly closed.

7.3. Specific end use(s)

Laboratory chemicals

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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

DNEL/DMEL values

CAS No	Substance	Exposure route	Effect	Value
111-27-3	hexan-1-ol			
Worker DNEL, long-term		inhalation	systemic	99 mg/m ³
Worker DNEL, long-term		inhalation	local	210 mg/m ³
Worker DNEL, long-term		dermal	systemic	28 mg/kg bw/day
Consumer DNEL, long-term		inhalation	systemic	24,5 mg/m ³
Consumer DNEL, long-term		dermal	systemic	14 mg/kg bw/day
Consumer DNEL, long-term		oral	systemic	14 mg/kg bw/day

PNEC values

CAS No	Substance	Value
111-27-3	hexan-1-ol	
Freshwater		0,51 mg/l
Freshwater (intermittent releases)		4 mg/l
Marine water		0,051 mg/l
Freshwater sediment		2,8 mg/kg
Marine sediment		0,28 mg/kg
Micro-organisms in sewage treatment plants (STP)		62 mg/l
Soil		0,25 mg/kg

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles
Face protection umbrella

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Trade name/designation: KCL 898 Butoject®

Recommended material: Butyl caoutchouc (butyl rubber) 0,7 mm

Wearing time with permanent contact: > 480 min

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By short-term hand contact

Trade name/designation: KCL 730 Camatril® Velours

Recommended material: NBR (Nitrile rubber) 0,4 mm

Wearing time with occasional contact (splashes): > 30 min

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).

Skin protection

Wear anti-static footwear and clothing

Wear fire resistant or flame retardant clothing.

Take off immediately all contaminated clothing and wash it before reuse.

Wash hands and face before breaks and after work and take a shower if necessary.

Respiratory protection

Wear breathing apparatus if exposed to vapours/dusts/aerosols.

Filtering device with filter or ventilator filtering device of type: A

Environmental exposure controls

Do not allow to enter into surface water or drains.

Danger of explosion

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid
Colour:	colourless
Odour:	characteristic
Odour threshold:	No data available
Melting point/freezing point:	-45 °C
Boiling point or initial boiling point and boiling range:	155 °C
Flammability:	No data available
Lower explosion limits:	1,2 vol. %
Upper explosion limits:	7,7 vol. %
Flash point:	60 °C
Auto-ignition temperature:	285 °C
Decomposition temperature:	No data available
pH-Value:	No data available
Viscosity / kinematic: (at 40 °C)	3,64 mm ² /s
Water solubility: (at 23 °C)	1,3 g/L
Solubility in other solvents	No data available
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	log Pow: 1,8
Dispersion stability:	No data available
Vapour pressure: (at 38 °C)	3,64 hPa
Vapour pressure: (at 20 °C)	1 hPa
Density:	0,82 g/cm ³

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Relative density:	No data available
Bulk density:	No data available
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information**Information with regard to physical hazard classes**

Explosive properties

In case of warming:

Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Sustaining combustion:

Sustaining combustion

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

No data available

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

Viscosity / dynamic:

0,592 mPa·s

(at 25 °C)

Flow time:

No data available

Further Information

No data available

SECTION 10: Stability and reactivity**10.1. Reactivity**

In case of warming:

Vapours may form explosive mixtures with air.

10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent, strong

Alkali metals

Alkaline earth metal

Aluminium

10.4. Conditions to avoid

Heat

10.5. Incompatible materials

Plastic articles

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

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SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

Harmful if swallowed.

Harmful in contact with skin.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
111-27-3	hexan-1-ol				
	oral	LD50 3210 mg/kg	Rat	Study report (1965)	OECD Guideline 401
	dermal	LD50 1500 - 2000 mg/kg	Rabbit	Study report (1977)	OECD Guideline 402

Irritation and corrosivity

Causes serious eye irritation.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Causes mild skin irritation.

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Based on available data, the classification criteria are not met.

STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Observe risk of aspiration if vomiting occurs.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards

Endocrine disrupting properties

No data available

Other information

No data available

Further information

Cough

Narcotic effects

Gastrointestinal complaints

Headache

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Irritant

SECTION 12: Ecological information

12.1. Toxicity

Based on available data, the classification criteria are not met.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
111-27-3	hexan-1-ol					
	Acute fish toxicity	LC50 97,2 - 97,5 mg/l	96 h	Pimephales promelas	In: Bishop WE, Cardwell RD, Heidolph BB	other: US EPA 1975
	Acute algae toxicity	ErC50 mg/l 79,7	72 h	Pseudokirchneriella subcapitata	Study report (2005)	OECD Guideline 201
	Acute crustacea toxicity	EC50 mg/l 123,6	48 h		Ecotoxicology and Environmental Safety 7	Method:
	Crustacea toxicity	NOEC mg/l 6,8 - 13	21 d	Daphnia magna	Ecotoxicology and Environmental Safety,	other: read-across and

12.2. Persistence and degradability

61,8 %; 30 d; aerob
OECD- 301D
Readily biodegradable (according to OECD criteria).

12.3. Bioaccumulative potential

log Pow: 1,8
No indication of bioaccumulation potential.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
111-27-3	hexan-1-ol	1,8

BCF

CAS No	Chemical name	BCF	Species	Source
111-27-3	hexan-1-ol	10		(2010)

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Do not allow to enter into surface water or drains.

Further information

Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.
Send to a physico-chemical treatment facility under observation of official regulations.

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Do not empty into drains.

Contaminated packaging

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number or ID number:	UN 2282
14.2. UN proper shipping name:	HEXANOLS
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	30
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number or ID number:	UN 2282
14.2. UN proper shipping name:	HEXANOLS
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Classification code:	F1
Limited quantity:	5 L
Excepted quantity:	E1

Marine transport (IMDG)

14.1. UN number or ID number:	UN 2282
14.2. UN proper shipping name:	HEXANOLS
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Special Provisions:	-
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 2282
14.2. UN proper shipping name:	HEXANOLS
14.3. Transport hazard class(es):	3
14.4. Packing group:	III
Hazard label:	3
Limited quantity Passenger:	10 L
Passenger LQ:	Y344
Excepted quantity:	E1
IATA-packing instructions - Passenger:	355
IATA-max. quantity - Passenger:	60 L
IATA-packing instructions - Cargo:	366
IATA-max. quantity - Cargo:	220 L

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

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14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3, Entry 40, Entry 75

Information according to 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

Additional information

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 = 0.1 % (w/w).

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 1 - slightly hazardous to water

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 12.

Abbreviations and acronyms

Flam. Liq: Flammable liquid

Acute Tox: Acute toxicity

Eye Irrit: Eye irritation

Relevant H and EUH statements (number and full text)

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H302+H312 Harmful if swallowed or in contact with skin.

H312 Harmful in contact with skin.

H319 Causes serious eye irritation.

Further Information

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material. The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.