

Safety Data Sheet

according to Regulation (EC) No 1907/2006

1-Octanol > 98.5 % for synthesis

Revision date: 21.09.2023

Product code: 12994

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

1.1. Product identifier

1-Octanol > 98.5 % for synthesis

REACH Registration Number: 01-2119486978-10-XXXX

CAS No: 111-87-5

EC No: 203-917-6

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

Telefax: 0203/5194-290

E-mail: info@analytichem.de

Contact person: Abteilung Produktsicherheit

Telephone: 0203/5194-107/117

E-mail: produktsicherheit@analytichem.de

Internet: www.analytichem.de

Responsible Department: Abteilung Produktsicherheit

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

Eye Irrit. 2; H319

Aquatic Chronic 3; H412

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning

Pictograms:



Hazard statements

H319

Causes serious eye irritation.

H412

Harmful to aquatic life with long lasting effects.

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Precautionary statements

P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients**3.1. Substances**

Sum formula:	CH ₃ (CH ₂) ₇ OH
Molecular weight:	130,23 g/mol

Hazardous components

CAS No	Chemical name	Quantity		
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
111-87-5	octan-1-ol			100 %
	203-917-6		01-2119486978-10-XXXX	
	Eye Irrit. 2, Aquatic Chronic 3; H319 H412			

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			
111-87-5	203-917-6	octan-1-ol	100 %	
	dermal: LD50 = 2000 - 4000 mg/kg; oral: LD50 = > 5000 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.

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.

Consult an ophthalmologist.

After ingestion

Observe risk of aspiration if vomiting occurs.

Call a physician immediately.

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

Cough, Narcotic effects
Gastrointestinal complaints, Headache
Irritant, Dizziness
May cause drowsiness or dizziness.
Agitation, Spasms

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.

Additional information

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

For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
Emergency procedures
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.

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).

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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.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

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

Hints on joint storage

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

Further information on storage conditions

storage temperature: +5°C - +30°C

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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PNEC values

CAS No	Substance	
Environmental compartment		Value
111-87-5	octan-1-ol	
Freshwater		0,2 mg/l
Marine water		0,02 mg/l
Freshwater sediment		2,1 mg/kg
Marine sediment		0,21 mg/kg
Micro-organisms in sewage treatment plants (STP)		55,5 mg/l
Soil		1,6 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 730 Camatril® Velours
Recommended material: NBR (Nitrile rubber) 0,4 mm
Wearing time with permanent contact: > 480 min

By short-term hand contact

Trade name/designation: KCL 720 Camapren®
Recommended material: CR (polychloroprene, chloroprene rubber) 0,65 mm
Wearing time with occasional contact (splashes): > 240 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.

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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:		No data available
Boiling point or initial boiling point and boiling range:		195 °C
Flammability:		No data available
Lower explosion limits:		0,8 vol. %
Upper explosion limits:		No data available
Flash point:		86 °C
Auto-ignition temperature:		270 °C
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic: (at 40 °C)		5,6 mm ² /s
Water solubility:		No data available
Solubility in other solvents		No data available
Dissolution rate:		No data available
Partition coefficient n-octanol/water:		log Pow: 3,5
Dispersion stability:		No data available
Vapour pressure: (at 20 °C)		0,031 hPa
Vapour pressure:		No data available
Density (at 20 °C):		0,83 g/cm ³
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: No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate: No data available

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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: (at 20 °C)	9 mPa·s
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
Acid

10.4. Conditions to avoid

Heat

10.5. Incompatible materials

Plastic articles
Rubber articles

10.6. Hazardous decomposition products

SECTION 5: Firefighting measures

Further information

No data available

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

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

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
111-87-5	octan-1-ol				
	oral	LD50 > 5000 mg/kg	Rat	Study report (1981)	OECD Guideline 401
	dermal	LD50 2000 - 4000 mg/kg	Rabbit	Study report (1976)	Method: other: contract laboratory proto

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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
Irritant, Dizziness
May cause drowsiness or dizziness.
Agitation, Spasms

SECTION 12: Ecological information

12.1. Toxicity

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
111-87-5	octan-1-ol					
	Acute fish toxicity	LC50 mg/l	13,3	96 h	Pimephales promelas	Aquatic Toxicology 6: 307-322 (1985) other: ASTM 1980
	Acute crustacea toxicity	EC50	25 mg/l	48 h		Ecotoxicology and Environmental Safety 7 Method:
	Crustacea toxicity	NOEC	1 mg/l	21 d	Daphnia magna	Wat. Res. 23(4): 501-510 (1989) other: Federal Environment Agency

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12.2. Persistence and degradability

92 %; 28 d; aerob
OECD 310
Readily biodegradable (according to OECD criteria).

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
111-87-5	octan-1-ol	3,5

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.
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.
No data available

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.
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: No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es): No dangerous good in sense of this transport regulation.
14.4. Packing group: No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

14.1. UN number or ID number: No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es): No dangerous good in sense of this transport regulation.
14.4. Packing group: No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

14.1. UN number or ID number: No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es): No dangerous good in sense of this transport regulation.
14.4. Packing group: No dangerous good in sense of this transport regulation.

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Air transport (ICAO-TI/IATA-DGR)

- 14.1. UN number or ID number:** No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es): No dangerous good in sense of this transport regulation.
14.4. Packing group: No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

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

Information according to 2012/18/EU Not subject to 2012/18/EU (SEVESO III)
(SEVESO III):

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).

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

SECTION 16: Other information

Abbreviations and acronyms

Eye Irrit: Eye irritation

Aquatic Chronic: Chronic aquatic hazard

Relevant H and EUH statements (number and full text)

H319 Causes serious eye irritation.

H412 Harmful to aquatic life with long lasting effects.

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.