

SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 06/17/2017

Version 1.5

SECTION 1. Identification

Product identifier

Product number	820931
Product name	1-Octanol for synthesis
CAS-No.	111-87-5

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

Identified uses	Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) MilliporeSigma is a business of Merck KGaA, Darmstadt, Germany.
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 4, H227

Eye irritation, Category 2A, H319

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

GHS-Labeling

Hazard pictograms



Signal Word

Warning

Hazard Statements

H227 Combustible liquid.

H319 Causes serious eye irritation.

Precautionary Statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

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P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face 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.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P235 Store in a well-ventilated place. Keep cool.
P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$\text{CH}_3(\text{CH}_2)_7\text{OH}$	$\text{C}_8\text{H}_{18}\text{O}$ (Hill)
Molar mass	130.23 g/mol	

Hazardous ingredients

Chemical name (Concentration)

CAS-No.

1-octanol ($\geq 90\%$ - $\leq 100\%$)

111-87-5

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

Skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

Eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

Ingestion

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis. irritant effects, CNS disorders, somnolence, Vertigo, euphoria, agitation, spasms

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. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Advice for firefighters

Special protective equipment for fire-fighters

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.

Suppress (knock down) gases/vapors/mists with a water spray jet. Remove container from danger zone and cool with water.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact.

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.

Environmental precautions

Do not let product enter drains.

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.

SECTION 7. Handling and storage

Precautions for 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.

Conditions for safe storage, including any incompatibilities

Tightly closed.

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Store below +30°C (+86°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0.40 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0.65 mm
Break through time:	> 240 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 730 Camatril® -Velours (full contact), KCL 720 Camapren® (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 and supplied by us as well as to the purpose specified by us. 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:

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapors/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapors of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are performed according to the instructions of the producer. These measures have to be properly documented.

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SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	characteristic
Odor Threshold	No information available.
pH	No information available.
pour point	ca. 3 - 7 °F (-16 - -14 °C)
	at 1,013 hPa Method: ISO 3016
Boiling point/boiling range	383 °F (195 °C) at 1,013 hPa
Flash point	ca. 187 °F (86 °C) Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	0.8 %(V)
Upper explosion limit	No information available.
Vapor pressure	0.031 hPa at 68 °F (20 °C)
Relative vapor density	4.5
Density	0.83 g/cm ³ at 68 °F (20 °C)
Relative density	No information available.
Water solubility	ca.0.43 g/l at 77 °F (25 °C) (External MSDS)
Partition coefficient: n-octanol/water	log Pow: 2.8 (experimental) (IUCILID) Bioaccumulation is not expected.
Autoignition temperature	No information available.

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Decomposition temperature	No information available.
Viscosity, dynamic	9.0 mPa.s at 68 °F (20 °C)
Explosive properties	Not classified as explosive.
Oxidizing properties	none
Ignition temperature	518 °F (270 °C) Method: DIN 51794
Viscosity, kinematic	ca.5.6 mm ² /s at 104 °F (40 °C) Method: ASTM D 445

SECTION 10. Stability and reactivity

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.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with:

Acid chlorides, Acid anhydrides, Oxidizing agents, acids, halogen compounds

Risk of explosion with:

perchloric acid, perchlorates

Conditions to avoid

Strong heating.

Incompatible materials

rubber, various plastics

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Eye contact, Skin contact

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Acute oral toxicity

LD50 Rat: > 5,000 mg/kg
OECD Test Guideline 401

Symptoms: Nausea, Vomiting, Gastrointestinal discomfort, Risk of aspiration upon vomiting.,
Pulmonary failure possible after aspiration of vomit.

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 Rabbit: > 2,000 - 4,000 mg/kg
OECD Test Guideline 402

Skin irritation

human
Result: No irritation
Patch Test 24 Hrs.

Eye irritation

Rabbit
Result: Severe irritations
OECD Test Guideline 405

Causes serious eye irritation.

Sensitization

Patch test:
Result: negative
Method: OECD Test Guideline 406

Genotoxicity in vivo

In vivo micronucleus test
Mouse
Result: negative
Method: OECD Test Guideline 474

Genotoxicity in vitro

Ames test
Salmonella typhimurium
Result: negative
Method: OECD Test Guideline 471
In vitro mammalian cell gene mutation test
MOUSE LYMPHOMA TEST
Result: negative
Method: OECD Test Guideline 476

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

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Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis.

After absorption of large quantities:

CNS disorders, somnolence, Dizziness, euphoria, agitation, Convulsions

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

flow-through test LC50 Pimephales promelas (fathead minnow): 13 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

Toxicity to algae

static test EC50 Desmodesmus subspicatus (green algae): 14 mg/l; 48 h

OECD Test Guideline 201

Toxicity to bacteria

EC50 activated sludge: 350 mg/l; 3 h

OECD Test Guideline 209

Toxicity to fish (Chronic toxicity)

flow-through test NOEC Pimephales promelas (fathead minnow): 1 - 10 mg/l; 7 d
(External MSDS)

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Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)
semi-static test NOEC Daphnia magna (Water flea): 1 mg/l; 21 d

Analytical monitoring: yes

OECD Test Guideline 211

Persistence and degradability

Biodegradability

92 %; 28 d; aerobic

OECD Test Guideline 310

Readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2.8

(experimental)

(IUCLID) Bioaccumulation is not expected.

Mobility in soil

No information available.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

Not classified as dangerous in the meaning of transport regulations.

Air transport (IATA)

Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

United States of America

SARA 313

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 302

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

Ingredients

1-octanol

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Labeling

Hazard pictograms



Signal Word

Warning

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Hazard Statements

H227 Combustible liquid.

H319 Causes serious eye irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary Statements

Prevention

P273 Avoid release to the environment.

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.

Full text of H-Statements referred to under sections 2 and 3.

H227 Combustible liquid.

H319 Causes serious eye irritation.

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.

Revision Date 06/17/2017

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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