Chemical Safety Data Sheet MSDS / SDS

1-Hexanol

Revision Date:2025-06-07 Revision Number:1

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

Product identifier

Product name	: 1-Hexanol
CBnumber	: CB8461421
CAS	: 111-27-3
EINECS Number	: 203-852-3
Synonyms	: 1-Hexanol,hexanol

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral

Label elements

Pictogram(s)

Signal word Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H302 Harmful if swallowed

H313 May be harmful in contact with skin

H319 Causes serious eye irritation

Precautionary statement(s)

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

P240 Ground/bond container and receiving equipment.

P241 Use explosion-proof electrical/ventilating/lighting/…/equipment.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-Hexanol
Synonyms	: 1-Hexanol,hexanol
CAS	: 111-27-3
EC number	: 203-852-3
MF	: C6H14O
MW	: 102.17

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest.

Following skin contact

Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink.

Most important symptoms and effects, both acute and delayed

Liquid causes eye burns and skin irritation. Breathing vapors is not expected to cause systemic illness. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

Basic Treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary . Monitor for pulmonary edema and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Higher alcohols (>3 carbons) and related compounds

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SECTION 5: Firefighting measures

Extinguishing media

Use carbon dioxide, dry chemical or "alcohol" foam extinguisher. Water is ineffective to fire fighting, but is effective to keep fire-exposed containers cool.

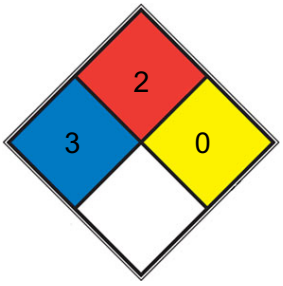
Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 129 [Flammable Liquids (Water-Miscible / Noxious)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Advice for firefighters

Use alcohol-resistant foam, dry powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

NFPA 704



■	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen, sulfuric acid, calcium hypochlorite, hexafluorosilicic acid)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in covered containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Absorb on paper. Evaporate on a glass or iron dish in hood. Burn the paper.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Above 63°C use a closed system and ventilation. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from strong oxidants.Protect containers against physical damage. Keep containers closed and store in well-ventilated, cool place.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Hexan-1-ol			
CAS No.	111-27-3			
	Limit value - Eight hours		**Limit value - Short term**	
	ppm	**mg/m^3**	**ppm**	**mg/m^3**
Germany (AGS)	50 (1)	210 (1)	50 (1)(2)	210 (1)(2)
	Remarks			
Germany (AGS)	(1) Inhalable aerosol and vapour (2) 15 minutes reference period			

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Liquid
Colour	Clear colorless
Odour	Characteristic; sweet alcohol; pleasant
Melting point/freezing point	-45 °C. Atm. press.:Ca. 1 atm.
Boiling point or initial boiling point and boiling range	155 °C. Atm. press.:101.59 kPa.
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	1.2-7.7%(V)
Flash point	60 °C. Atm. press.:Ca. 101.5 kPa.
Auto-ignition temperature	Ca. 313 °C. Atm. press.:Ca. 1 atm.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	kinematic viscosity (in mm2/s) = 3.64. Temperature:40°C.
Solubility	ethanol: soluble(lit.)
Partition coefficient n-octanol/water	log Pow = 1.8.
Vapour pressure	1 mm Hg (25.6 °C)
Density and/or relative density	0.823 g/cm3. Temperature:15.6 °C.
Relative vapour density	4.5 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with strong oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

Flammable liquid when exposed to heat, sparks or flame.HEXANOL is an alcohol. Flammable and/or toxic gases are generated by the combination of alcohols with alkali metals, nitrides, and strong reducing agents. They react with oxoacids and carboxylic acids to form esters plus water. Oxidizing agents convert them to aldehydes or ketones. Alcohols exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.

Conditions to avoid

no data available

Incompatible materials

Can react with oxidizing materials.

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - 3 210 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 21 mg/L air.
- Dermal: LD50 - rabbit (male/female) - 1 500 - 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the respiratory tract and skin. The substance is severely irritating to the eyes. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis.

STOT-repeated exposure

The substance defats the skin, which may cause dryness or cracking.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 97.2 - 97.5 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC0 - Daphnia magna - 152 mg/L - 24 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 79.7 mg/L - 72 h.

Toxicity to microorganisms: TT or EC3 - Pseudomonas putida - 62 mg/L - 16 h.

Persistence and degradability

AEROBIC: 5-Day theoretical BODs of 28%(1), 53% (initial concn of 100 ppm)(2) and 83.6% (initial concn of 2,000 ppm)(3) were observed for 1-hexanol in aerobic screening tests using a sewage inocula. An aerobic biodegradation rate constant of 7.99X10-2 1/hr(4), which corresponds to a half-life of 0.36 days(SRC), was determined in an aerobic screening test at pH 7 and 25 deg C using an activated sludge inocula. In a similar screening test, the rate constant was measured to be 1.7X10-2 1/hr(5), which corresponds to a biodegradation half-life of 1.7 days(SRC).

Bioaccumulative potential

An estimated BCF of 21 was calculated for 1-hexanol(SRC), using a log Kow of 2.03(1) and regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

A Koc of 10.2 was determined for 1-hexanol on a Hagerstown silt loam soil(1). According to a suggested classification scheme(2), this Koc value suggests that 1-hexanol is expected to have very high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/

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