

Chemical Safety Data Sheet MSDS / SDS

Hexane-1,6-diol SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: Hexane-1,6-diol

CAS: 629-11-8

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.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Not classified.

GHS label elements, including precautionary statements

Signal word No signal word

Hazard statement(s)

none

Precautionary statement(s)**Prevention**

none

Response

none

Storage

none

Disposal

none

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients**Substance**

Chemical name: Hexane-1,6-diol

Common names and
synonyms: Hexane-1,6-diol

CAS number: 629-11-8

EC number: 211-074-0

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

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. Give one or two glasses of water to drink.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Higher alcohols (>3 carbons) and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

To fight fire use foam, CO₂, dry chemical

Specific hazards arising from the chemical

Combustible. Finely dispersed particles form explosive mixtures in air.

Special protective actions for fire-fighters

Use alcohol-resistant foam, powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

Environmental precautions

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. 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.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Solid. Crystalline.

Colour: Colorless.

Odour: no data available

Melting point/freezing point: 39.5 - 42.1 °C.

Boiling point or initial boiling point and boiling range:	250 °C. Atm. press.:1 013 hPa.
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	136 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature:	320 °C. Atm. press.:1 013.25 hPa.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 61. Temperature:43.0°C. Remarks:Slightly above melting point.
Solubility:	Sol in water, alcohol, sparingly soluble in hot ether.
Partition coefficient n-octanol/water:	log Pow = 0. Temperature:25 °C.
Vapour pressure:	0.001 hPa. Temperature:25 °C. Remarks:Estimated.
Density and/or relative density:	0.96 g/cm ³ . Temperature:20 °C.
Relative vapour density:	4.07 (Air = 1)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts violently with oxidants.

Chemical stability

no data available

Possibility of hazardous reactions

Moderate when exposed to heat or flame. Dust explosion possible if in powder or granular form, mixed with air.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 - rat (male/female) - ca. 3 000 mg/kg bw.

Inhalation: LC0 - rat (male/female) - 3.3 mg/L air.

Dermal: LD50 - rabbit (male/female) - > 2 500 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 eyes.

STOT-repeated exposure

no data available

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 - *Leuciscus idus* - 4 640 - 10 000 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - > 500 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 5 940 mg/L - 72 h.

Toxicity to microorganisms: EC10 - *Pseudomonas putida* - 8 400 mg/L - 17 h.

Persistence and degradability

AEROBIC: 1,6-Hexanediol, present at 20 mg dissolved organic carbon/L, reached between 91 and 98% of its theoretical CO₂ evolution in 28 days using a modified Sturm test(1). Using a modified OECD screening test, 1,6-hexanediol reached between 94 and 96% dissolved organic carbon removal after 28 days(1).

Bioaccumulative potential

An estimated BCF of 3.2 was calculated for 1,6-hexanediol(SRC), using an estimated log K_{ow} of 0.76(1) and a 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

Using a structure estimation method based on molecular connectivity indices(1), the K_{oc} of 1,6-hexanediol can be estimated to be less than 1(SRC). According to a classification scheme(2), this estimated K_{oc} value suggests that 1,6-hexanediol 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/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any