

Chemical Safety Data Sheet MSDS / SDS

Heptanoic acid 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: Heptanoic acid

CAS: 111-14-8

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**

Skin corrosion, Sub-category 1B

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H314 Causes severe skin burns and eye damage

Precautionary statement(s)

Prevention

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P264 Wash ... thoroughly after handling.

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

Response

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

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

Storage

P405 Store locked up.

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Heptanoic acid
Common names and synonyms:	Heptanoic acid
CAS number:	111-14-8
EC number:	203-838-7
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

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. Do NOT induce vomiting. Give one or two glasses of water to drink. Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Harmful if swallowed, inhaled, or absorbed through skin. Extremely destructive to mucous membranes, upper respiratory tract, skin, and eyes. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis, and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. (USCG, 1999)

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

FIRST AID ... Inhalation-Fresh air, rest. Half-upright position. Artificial respiration if indicated. Refer for medical attention; Skin-

Remove contaminated clothes. Rinse skin with plenty of water or shower; Eyes-First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then take to a doctor; Ingestion-Rinse mouth. Do NOT induce vomiting. Give plenty of water to drink. Rest. Refer for medical attention ... The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation is therefore essential.

SECTION 5: Firefighting measures

Suitable extinguishing media

FIRE FIGHTING /with/ Powder, water spray, foam, carbon dioxide.

Specific hazards arising from the chemical

This chemical is probably combustible. (NTP, 1992)

Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: complete protective clothing including self-contained breathing apparatus. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. Personal protection: complete protective clothing including self-contained breathing apparatus.

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. See Chemical Dangers. 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 bases and food and feedstuffs. Separated from bases, food and feedstuffs.

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 face shield or eye protection in combination with breathing protection.

Skin protection

Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid. Oily.
Colour:	Clear.
Odour:	Disagreeable, rancid odor; faint tallow-like odor when spectroscopically pure.
Melting point/freezing point:	-8 °C. Atm. press.:1.013 hPa. Remarks:As no information are given for the atmospheric pressure it is assumed to be at normal pressure.
Boiling point or initial boiling point and boiling range:	223 °C. Atm. press.:760 mm Hg.
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	117 °C. Atm. press.:101.3 kPa.
Auto-ignition temperature:	275 °C. Atm. press.:999 mBar.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 3.4. Temperature:30.0°C. Remarks:The data is indicated in cP. The conversion factor is 1 cP=1 mPa.s.;dynamic viscosity (in mPa s) = 0.82. Temperature:120.0°C. Remarks:The data is indicated in cP. The conversion factor is 1 cP=1 mPa.s.
Solubility:	Partially miscible with water

Partition coefficient n-octanol/water:	log Pow = 2.54. Temperature:20 °C.
Vapour pressure:	1.349 Pa. Temperature:20 °C.;2.201 Pa. Temperature:25 °C.
Density and/or relative density:	0.92. Temperature:20 °C.
Relative vapour density:	4.5 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Slightly soluble in water.

Chemical stability

no data available

Possibility of hazardous reactions

CombustibleHEPTANOIC ACID reacts exothermically with bases. Can react, particularly if moist, with active metals to form gaseous hydrogen and a metal salt. Such reactions are slow if the acid remains dry. Corrodes or dissolves iron, steel, and aluminum parts and containers under ordinary conditions. Reacts with cyanide salts to generate gaseous hydrogen cyanide, particularly if moist. May generate flammable and/or toxic gases with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Reacts with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Reacts exothermically with carbonates and bicarbonates to generate a harmless gas (carbon dioxide). Can be oxidized exothermically by strong oxidizing agents and reduced exothermically by strong reducing agents. A wide variety of products is possible. May initiate polymerization reactions; may catalyze chemical reactions.

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) - 8 370 mg/kg bw. Remarks:SD +/- 1203 mg/kg.

Inhalation: LC50 - rat (male/female) - > 4.6 mg/L air (analytical).

Dermal: LD50 - rabbit (male/female) - > 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 corrosive to the eyes, skin and respiratory tract. Inhalation of high concentrations may cause lung oedema, but only after initial corrosive effects on the eyes and the upper respiratory tract have become manifest. See Notes. The effects may be delayed. Medical observation is indicated.

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 - *Pimephales promelas* - > 92 mg/L - 96 h. Remarks: / subjective assessments were also made on the type and incidence of sub-lethal effects compared with control fish.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 859.6 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata* (previous names: *Raphidocelis subcapitata*, *Selenastrum capricornutum*) - 61.2 mg/L - 72 h.

Toxicity to microorganisms: EC10 - *Pseudomonas putida* - > 1 000 mg/L - 17 h.

Persistence and degradability

AEROBIC: Heptanoic acid reached 44, 61, 54, and 58% of its theoretical BOD after 2, 5, 10, and 30 days, respectively, using a domestic sewage inoculum and a heptanoic acid concn of 3.1 ppm(1). Heptanoic acid, present at an initial concn of 500 ppm, was degraded 24.6, 36.1, and 49.2% of its theoretical BOD after 72 hours, by activated sludge obtained from three different treatment plants(2). In a Warburg test using an activated sludge inoculum acclimated to phenol, heptanoic acid, present at a concn of 500 ppm, reached 27% of its theoretical BOD after 12 hours(3). A 99% BOD reduction was observed for heptanoic acid after 16 days using an activated sludge system operated under semi-continuous conditions(4). In Warburg respirometer tests using an activated sludge seed, heptanoic acid, present at a concn of 500 ppm, reached 12.8, 25.4, and 42.6% of its theoretical oxygen demand after 6, 12, and 24 hours incubation, respectively(5). A total organic carbon removal ratio of 96% was observed for heptanoic acid using a non-acclimated activated sludge and an initial heptanoic acid concn of 100 mg total organic carbon/L(6).

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for heptanoic acid(SRC), using a log Kow of 2.42(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

The Koc of undissociated heptanoic acid is estimated as 490(SRC), using a log Kow of 2.42(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that undissociated heptanoic acid is expected to have moderate mobility in soil. The pKa of heptanoic acid is 4.8(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

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: UN3265 (For reference only, please check.)

IMDG: UN3265 (For reference only, please check.)

IATA: UN3265 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

IATA: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (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

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/>

Other Information

The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential. Isolate contaminated clothing by sealing in a bag or other container.

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