SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0
Creation Date: July 15, 2019
Revision Date: July 15, 2019

SECTION 1: Identification

1.1 GHS Product identifier

Product name Hexanoic acid

1.2 Other means of identification

Product number -
Other names Caproic acid; n-Caproic acid; n-Hexoic acid

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.
Uses advised against no data available

1.4 Supplier's details

Company Shanghai Baishun Biotechnology Co., Ltd
Address No. 26, Lane 918, Lianye Road, Zhelin Town, Fengxian District, Shanghai, 201400, China
Telephone +86-21-37581181

1.5 Emergency phone number

Emergency phone number +86-21-37581181
Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Skin corrosion, Sub-category 1C

2.2 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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Hexanoic acid	Hexanoic acid	142-62-1	205-550-7	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

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.

4.2 Most important symptoms/effects, acute and delayed

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

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

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist respirations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . Monitor for shock 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. Activated charcoal is not effective . Do not attempt to neutralize because of exothermic reaction. Cover skin burns with dry, sterile dressings after decontamination . Organic acids and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

To fight fire use, CO2, dry chemical, fog, mist.

5.2 Specific hazards arising from the chemical

Special Hazards of Combustion Products: Irritating vapor may be generated. (USCG, 1999)

5.3 Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

6.2 Environmental precautions

Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

6.3 Methods and materials for containment and cleaning up

Collect leaking liquid in sealable containers. Wash away spilled liquid with plenty of water. Do NOT wash away into sewer.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames. NO contact with strong oxidizing agents. 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.

7.2 Conditions for safe storage, including any incompatibilities

Separated from strong oxidants, strong bases and food and feedstuffs.Separated from strong oxidants, strong bases, food and feedstuffs.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Component	Hexanoic acid			
CAS No.	142-62-1			
	Limit value - Eight hours		**Limit value - Short term**	
	ppm	**mg/m^3**	**ppm**	**mg/m^3**
Latvia		5		
	Remarks			

Biological limit values

no data available

8.2 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.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. 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.
Colour	Oily liquid
Odour	Characteristic goat-like odor
Melting point/freezing point	-6 °C. Atm. press.:Ca. 1 013 hPa.
Boiling point or initial boiling point and boiling range	202.8 °C. Atm. press.:1 013 hPa.
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	Lower flammable limit: 1.3% by volume; Upper flammable limit: 9.3% by volume
Flash point	110 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature	380 °C. Atm. press.:Ca. 1 013 hPa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	dynamic viscosity (in mPa s) = 3.2. Temperature:20°C.
Solubility	Partially miscible with water
Partition coefficient n-octanol/water	log Pow = 2.05.
Vapour pressure	0.043 mm Hg. Temperature:25 °C. Remarks:0.058 hPa.
Density and/or relative density	0.93 g/cm³. Temperature:20 °C.
Relative vapour density	4 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

The substance is a weak acid. Reacts violently with acids, strong bases and oxidants.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

CAPROIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are

accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Carboxylic acids with six or fewer carbon atoms are freely or moderately soluble in water; those with more than six carbons are slightly soluble in water. Soluble carboxylic acid dissociate to an extent in water to yield hydrogen ions. The pH of solutions of carboxylic acids is therefore less than 7.0. Many insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H2S and SO3), dithionites (SO2), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions. This compound reacts with bases, oxidizing agents and reducing agents. (NTP, 1992).

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Can react with oxidizing materials.

10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male) - 6 440 mg/kg bw. Remarks:Estimated value/range.
- Inhalation: LC50 - rat (male) - > 1.368 mg/L air (nominal).
- Dermal: LD50 - rat (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 irritating to the eyes, skin and respiratory tract. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis.

STOT-repeated exposure

See Notes.

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - Pimephales promelas - 88 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 72 mg/L - 48 h.
- Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 52.3 mg/L - 72 h.
- Toxicity to microorganisms: EC10 - Pseudomonas putida - 912 mg/L - 18 h.

12.2 Persistence and degradability

AEROBIC: A 5-day theoretical BOD of 44% was observed for hexanoic acid in an aerobic screening test using a sewage inoculum(1). Five and 20-day theoretical BODs of 66 and 87% were observed in another aerobic screening test using a sewage inoculum(2). Using a Warburg respirometer, an adapted sewage inoculum and 10,000 ppm concns of hexanoic acid, respective 5-, 10- and 20-day theoretical BODs of 29, 66 and 69% were measured under aerobic conditions(3). One-day theoretical BODs of 26-54% were determined in a Warburg respirometer using various activate sludge inocula(4). Five-day theoretical BODs of 98-99% were achieved in an aerobic screening study using acclimated activated sludge inoculum(5). Respective 2-, 5-, 10- and 30-day theoretical BODs of 42, 48, 54 and 65% were measured in an aerobic Warburg respirometer study using sewage inoculum(6). Using a Warburg respirometer and activated sludge inocula from three Tennessee municipal plants, theoretical BODs of 34.9-61.2% were measured over a 3-day inoculation period(7).

12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated for hexanoic acid(SRC), using a log Kow of 1.92(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).

12.4 Mobility in soil

Koc values of 26, 24 and 37 have been experimentally measured, for an acidic forest soil (pH 2.8, 4.85% organic carbon), agricultural soil (pH 6.7, 1.25% organic carbon), and a lake sediment (pH 7.1, 1.58% organic carbon), respectively(1). According to a classification scheme(2), these measured Koc values suggest that hexanoic acid is very highly mobile in soil(SRC). In addition, the pKa of hexanoic acid is 4.88(3), indicating that this compound will primarily exist as an anion in the environment, and anions generally possess high mobility in soil(4).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 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

14.1 UN Number

ADR/RID: UN2829 (For reference only, please check.)

IMDG: UN2829 (For reference only, please check.)

IATA: UN2829 (For reference only, please check.)

14.2 UN Proper Shipping Name

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

IMDG: CAPROIC ACID (For reference only, please check.)

IATA: CAPROIC ACID (For reference only, please check.)

14.3 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.)

14.4 Packing group, if applicable

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

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

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

14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Hexanoic acid	Hexanoic acid	142-62-1	205-550-7
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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

Creation Date	July 15, 2019
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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

Insufficient data are available on the effect of this substance on human health, therefore utmost care must be taken.

Any questions regarding this SDS, Please send your inquiry to sds@xixisys.com

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