

Chemical Safety Data Sheet MSDS / SDS

Hexanoic acid

Revision Date:2023-12-02 Revision Number:1

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

Product identifier

Product name : Hexanoic acid
CBnumber : CB3224164
CAS : 142-62-1
EINECS Number : 205-550-7
Synonyms : Hexanoic acid, Caproic Acid

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 : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P405 Store locked up.

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

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

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

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

Hazard statements

H331 Toxic if inhaled

H318 Causes serious eye damage

H314 Causes severe skin burns and eye damage

H311 Toxic in contact with skin
H302 Harmful if swallowed
H290 May be corrosive to metals

SECTION 3: Composition/information on ingredients

Substance

Product name	: Hexanoic acid
Synonyms	: Hexanoic acid, Caproic Acid
CAS	: 142-62-1
EC number	: 205-550-7
MF	: C ₆ H ₁₂ O ₂
MW	: 116.16

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides Combustible.

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

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 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

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

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 480 min

Material tested: Camatril? (KCL 730 / Aldrich Z677442, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,2 mm Break through time: 30 min

Material tested: Dermatril? P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved

gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	Stench.
Odour Threshold	0.0006ppm
pH	4 (1g/l, H ₂ O, 20 °C)
Melting point/freezing point	Melting point/range: -3 °C
Initial boiling point and boiling range	204 - 205 °C at 1.013 hPa
Flash point	102 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 10 %(V) Lower explosion limit: 2 %(V)
Vapour pressure	1 hPa at 72 °C 0,24 hPa at 20 °C
Vapour density	4,01 - (Air = 1.0)
Relative density	0.929 (20/4 °C)
Water solubility	10.300 mg/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 1,75 at 25 °C
Autoignition temperature	380 °C at 1.013 hPa
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Dissociation constant 4,88

Relative vapor density

4,01 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Bases, Oxidizing agents, Reducing agents, Allyl alcohol

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

No data available

LD50 Dermal - Rabbit - 584 mg/kg

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Mammal

Result: Corrosive - 10 min (OECD Test Guideline 437)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 orally in rats: 3.0 g/kg (Smyth, Carpenter)

SECTION 12: Ecological information

Toxicity

Toxicity to fish

static test LC50 - Pimephales promelas (fathead minnow) - 88 mg/l

- 96 h

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 84 % - Readily biodegradable. (OECD Test Guideline 301D)

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Harmful to aquatic life. Harmful to aquatic life.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 2829 IMDG: 2829 IATA: 2829

UN proper shipping name

ADR/RID: CAPROIC ACID IMDG: CAPROIC ACID IATA: Caproic acid

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

EC Inventory: Listed.

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

Korea Existing Chemicals List (KECL): Listed. website: <http://ncis.nier.go.kr>

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

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Other Information

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

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.