

SAFETY DATA SHEET

Version 6.12
Revision Date 03/07/2024
Print Date 06/23/2024

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

1.1 Product identifiers

Product name : Hexanoic acid

Product Number : 153745
Brand : Aldrich
CAS-No. : 142-62-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin corrosion (Category 1C), H314
Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 3), H402

For the full text of the H-Statements mentioned in this Section, see Section 16.

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2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H314

Causes severe skin burns and eye damage.

H402

Harmful to aquatic life.

Precautionary Statements

P264

Wash skin thoroughly after handling.

P273

Avoid release to the environment.

P280

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

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 +

P310

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P363

Wash contaminated clothing before reuse.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stenchr., Rapidly absorbed through skin.

Stenchr., Rapidly absorbed through skin.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Caproic acid
Acid C6

Formula : C₆H₁₂O₂
Molecular weight : 116.16 g/mol
CAS-No. : 142-62-1
EC-No. : 205-550-7

Component	Classification	Concentration
hexanoic acid	Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; H314, H318, H402 Concentration limits: > 60 %: 1C, ; 3 - 60 %: Eye Dam./Irrit. 1, ; 3 - 60	<= 100 %

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	%: 2, ; 1 - 3 %: Eye Dam./Irrit. 2, ; 1 - 3 %: 2, ;	
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For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

7.3 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

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

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

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

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)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	Stench.
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -3 °C (27 °F)
f) Initial boiling point and boiling range	204 - 205 °C 399 - 401 °F at 1,013 hPa
g) Flash point	102 °C (216 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 10 %(V) Lower explosion limit: 2 %(V)
k) Vapor pressure	1 hPa at 72 °C (162 °F) 0.24 hPa at 20 °C(68 °F)
l) Vapor density	4.01 - (Air = 1.0)
m) Density	0.927 g/cm ³
Relative density	No data available
n) Water solubility	10.3 g/l at 25 °C (77 °F) - completely soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.75 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	380 °C (716 °F) at 1,013 hPa
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

9.2 Other safety information

Dissociation constant	4.88
Relative vapor density	4.01 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong bases
Strong oxidizing agents
strong reducing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 3,000 mg/kg

Remarks: (RTECS)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: , damage of respiratory tract, After a latency period: , Inhalation may lead to the formation of oedemas in the respiratory tract.

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: sebacic acid

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 - Bovine cornea

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

Remarks: Causes serious eye damage.

Remarks: Lacrimal irritation due to vapours.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

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Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Carcinogenicity

- IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

11.2 Additional Information

RTECS: MO5250000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Nausea
Discomfort
shock
Unconsciousness
Changes in the blood count

Damage to:

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 88 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 72 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: heptanoic acid; oenanthic acid
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 56.4 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: heptanoic acid; oenanthic acid
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 17.9 mg/l - 21 d (OECD Test Guideline 211) Remarks: The value is given in analogy to the following substances: heptanoic acid; oenanthic acid

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 84 % - Readily biodegradable. (OECD Test Guideline 301D)
Ratio BOD/ThBOD	44 % Remarks: (Lit.)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information**DOT (US)**

UN number: 2829 Class: 8 Packing group: III
Proper shipping name: Caproic acid
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2829 Class: 8 Packing group: III EMS-No: F-A, S-B
Proper shipping name: CAPROIC ACID

IATA

UN number: 2829 Class: 8 Packing group: III
Proper shipping name: Caproic acid

SECTION 15: Regulatory information**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
hexanoic acid	142-62-1	

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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