SAFETY DATA SHEET

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

1.1 Product identifiers
Product name : Hexanoic acid
Product Number : W255904
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

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)
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 3), H311
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.

2.2 GHS Label elements, including precautionary statements
Pictogram

Aldrich - W255904
Signal Word
Danger

Hazard statement(s)
H302 Harmful if swallowed.
H311 Toxic in contact with skin.
H314 Causes severe skin burns and eye damage.
H402 Harmful to aquatic life.

Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
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.
P362 Take off contaminated clothing and wash 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
Stench., Rapidly absorbed through skin.
Stench., 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

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>hexanoic acid</td>
<td>Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; H314, H318, H402</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Aldrich - W255904
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
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 carefully 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 in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

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)

- **Splash contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.11 mm
  - Break through time: 30 min
  - Material tested: KCL 741 Dermatril® L

**Body Protection**

**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/cm³
   Relative density
   No data available

n) Water solubility
   10,300 mg/l at 25 °C (77 °F)

o) Partition coefficient: n-octanol/water
   log Pow: 1.75 at 25 °C (77 °F)

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
- Strong oxidizing agents

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
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

<table>
<thead>
<tr>
<th>Toxicity to fish</th>
<th>static test LC50 - Pimephales promelas (fathead minnow) - 88 mg/l - 96 h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remarks:</td>
<td>(ECHA)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Toxicity to daphnia and other aquatic invertebrates</th>
<th>semi-static test EC50 - Daphnia magna (Water flea) - 72 mg/l - 48 h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remarks: The value is given in analogy to the following substances:</td>
<td>heptanoic acid; oenanthic acid</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Toxicity to algae</th>
<th>static test ErC50 - Pseudokirchneriella subcapitata - 56.4 mg/l - 72 h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remarks: The value is given in analogy to the following substances:</td>
<td>heptanoic acid; oenanthic acid</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)</th>
<th>semi-static test NOEC - Daphnia magna (Water flea) - 17.9 mg/l - 21 d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remarks: The value is given in analogy to the following substances:</td>
<td>heptanoic acid; oenanthic acid</td>
</tr>
</tbody>
</table>

### 12.2 Persistence and degradability

<table>
<thead>
<tr>
<th>Biodegradability</th>
<th>aerobic - Exposure time 28 d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result:</td>
<td>84 % - Readily biodegradable.</td>
</tr>
<tr>
<td>(OECD Test Guideline 301D)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ratio BOD/ThBOD</th>
<th>44 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Remarks:</td>
<td>(Lit.)</td>
</tr>
</tbody>
</table>

### 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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>hexanoic acid</td>
<td>142-62-1</td>
<td></td>
</tr>
</tbody>
</table>
SECTION 16: Other information

Further information
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. 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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