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

1.1 Product identifiers

Product name : 4-Methylvaleric acid

Product Number : 277827
Brand : Aldrich
CAS-No. : 646-07-1

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)

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

Signal Word : Danger
Hazard statement(s)
H314 Causes severe skin burns and eye damage.
H402 Harmful to aquatic life.

Precautionary statement(s)
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 - none

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>4-Methylpentanoic acid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Isocaproic acid</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₆H₁₂O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>116.16 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>646-07-1</td>
</tr>
<tr>
<td>EC-No.</td>
<td>211-464-0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-methylvaleric acid</td>
<td>Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; H314, H318, H402</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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**
Carbon dioxide (CO2) Foam 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: 60 min
Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic
compounds
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.

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**SECTION 9: Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

| a) Appearance | Form: clear, liquid |
| b) Odor | No data available |
9.2 Other safety information
No data available

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:

Aldrich - 277827

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
alkalines
Strong oxidizing 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 - 2,050 mg/kg
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Remarks: (RTECS)
Inhalation: No data available
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: hexanoic acid
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)
Remarks: The value is given in analogy to the following substances: hexanoic acid

Serious eye damage/eye irritation
Eyes - Bovine cornea
Result: Corrosive - 10 min
(OECD Test Guideline 437)
Remarks: The value is given in analogy to the following substances: hexanoic acid
Remarks: Causes serious eye damage.

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

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: NR2975000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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)
The value is given in analogy to the following substances: hexanoic acid

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

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: 3265   Class: 8   Packing group: III
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (4-methylvaleric acid)

Aldrich - 277827
Reportable Quantity (RQ): Poison Inhalation Hazard: No

**IMDG**
- UN number: 3265
- Class: 8
- Packing group: III
- EMS-No: F-A, S-B
- Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (4-methylvaleric acid)

**IATA**
- UN number: 3265
- Class: 8
- Packing group: III
- Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (4-methylvaleric 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.

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

**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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