

SAFETY DATA SHEET

Version 6.8
Revision Date 05/24/2023
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 4-Methylpentanoic acid

Product Number : W346306

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

| | |
|------------------|---|
| Synonyms | : 4-Methylvaleric acid 4-Methylpentanoic acid Isocaproic acid |
| Formula | : C ₆ H ₁₂ O ₂ |
| Molecular weight | : 116.16 g/mol |
| CAS-No. | : 646-07-1 |
| EC-No. | : 211-464-0 |

| Component | Classification | Concentration |
|-----------------------------|--|---------------|
| 4-methylvaleric acid | | |
| | Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; H314, H318, H402 | <= 100 % |

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. Chemisorb®). 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 EN374 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 EN374 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

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 |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point: -33 °C (-27 °F) |
| f) Initial boiling point and boiling range | 199 - 201 °C 390 - 394 °F - lit. |
| g) Flash point | 97 °C (207 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, | No data available |

| | | |
|----|--|---|
| | gas) | |
| j) | Upper/lower flammability or explosive limits | No data available |
| k) | Vapor pressure | No data available |
| l) | Vapor density | No data available |
| m) | Density | 0.923 g/cm ³ at 25 °C (77 °F) - lit. |
| | Relative density | No data available |
| n) | Water solubility | No data available |
| o) | Partition coefficient: n-octanol/water | No data available |
| p) | Autoignition temperature | No data available |
| 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

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:

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 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: hexanoic acid 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: 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: |
|------------------|--|

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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)
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.

SARA 311/312 Hazards

Acute Health Hazard

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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