

## SAFETY DATA SHEET

Version 6.4  
Revision Date 08/28/2020  
Print Date 12/09/2021**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)**

Acute toxicity, Dermal (Category 3), H311

Skin corrosion (Category 1C), H314

Serious eye damage (Category 1), H318

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)

H311

Toxic in contact with skin.

H314	Causes severe skin burns and eye damage.
Precautionary statement(s)	
P264	Wash skin thoroughly after handling.
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.
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 - none

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : 4-Methylvaleric acid  
4-Methylpentanoic acid  
Isocaproic acid

Formula : C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>  
Molecular weight : 116.16 g/mol  
CAS-No. : 646-07-1  
EC-No. : 211-464-0

Component	Classification	Concentration
<b>4-methylvaleric acid</b>	Acute Tox. 3; Skin Corr. 1C; Eye Dam. 1; H311, H314, H318	<= 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 aider needs to protect himself. 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 (CO<sub>2</sub>) 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 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

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic 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](http://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](http://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, gas)                    | No data available                        |
| j) Upper/lower flammability or explosive limits | No data available                        |
| k) Vapor pressure                               | No data available                        |
| l) Vapor density                                | No data available                        |
| m) Relative density                             | 0.923 g/cm <sup>3</sup> at 25 °C (77 °F) |
| 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 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

No data available

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents, Strong bases

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides  
Other decomposition products - No data available  
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

Remarks: (RTECS)

Inhalation: No data available

LD50 Dermal - Rabbit - 966 mg/kg

Remarks: (RTECS)

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### 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

Acute oral toxicity - If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

#### **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**

No data available

### **12.2 Persistence and degradability**

No data available

### **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 Other adverse effects**

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Discharge into the environment must be avoided.

---

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

Waste material must be disposed of in accordance with the national and local No mixing with other waste. Handle uncleaned containers like the product. See [www.retrologistik.com](http://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: 2922 Class: 8 (6.1) Packing group: II  
Proper shipping name: Corrosive liquids, toxic, n.o.s. (4-methylvaleric acid)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 2922 Class: 8 (6.1) Packing group: II EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE LIQUID, TOXIC, N.O.S. (4-methylvaleric acid)

**IATA**

UN number: 2922 Class: 8 (6.1) Packing group: II  
Proper shipping name: Corrosive liquid, toxic, 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.

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

4-methylvaleric acid	CAS-No. 646-07-1	Revision Date
----------------------	---------------------	---------------

**New Jersey Right To Know Components**

4-methylvaleric acid	CAS-No. 646-07-1	Revision Date
----------------------	---------------------	---------------



---

## 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.4

Revision Date: 08/28/2020

Print Date: 12/09/2021