

ALFAAA15405

## 4-Methylvaleric acid

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**产品说明:**  
**Product Description:** 4-甲基戊酸  
4-Methylvaleric acid

**Cat No. :** A15405  
**Synonyms** 4-Methylpentanoic acid; Isocaproic acid  
**CAS No** 646-07-1  
**Molecular Formula** C6 H12 O2

**Supplier** Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

**Emergency Telephone Number** For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Liquid

**Appearance**  
Clear

**Odor**  
pungent

#### Emergency Overview

May be harmful if swallowed. Toxic in contact with skin. Causes severe skin burns and eye damage.

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 5
Acute Dermal Toxicity	Category 3
Skin Corrosion/Irritation	Category 1 C
Serious Eye Damage/Eye Irritation	Category 1

#### Label Elements



**Signal Word**

**Danger**

## 4-Methylvaleric acid

**Hazard Statements**

H303 - May be harmful if swallowed

H311 - Toxic in contact with skin

H314 - Causes severe skin burns and eye damage

**Precautionary Statements****Prevention**

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310 - Immediately call a POISON CENTER or doctor

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 or shower

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P405 - Store locked up

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

May be harmful if swallowed. Toxic in contact with skin. Corrosive. Causes skin and eye burns.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil. The product is insoluble and floats on water. The product evaporates slowly.

Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
Isohexanoic acid	646-07-1	>95

**SECTION 4. FIRST AID MEASURES****General Advice**

Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Inhalation**

Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Remove to fresh air. Immediate medical attention is required. If not breathing, give artificial respiration.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

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**Most important symptoms and effects**

Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Use personal protective equipment as required. Ensure adequate ventilation.

**Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Use only under a chemical fume hood. Wear personal protective equipment/face protection.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place. Corrosives area.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

## 4-Methylvaleric acid

**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

**Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber Butyl rubber Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Long sleeved clothing

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Particulates filter conforming to EN 143 Acid gases filter Type E Yellow conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** No information available.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

**Appearance** Clear  
**Physical State** Liquid

## 4-Methylvaleric acid

Odor	pungent	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-35 °C / -31 °F	
Softening Point	No data available	
Boiling Point/Range	200 °C / 392 °F	@ 760 mmHg
Flash Point	97 °C / 206.6 °F	<b>Method -</b> No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No information available	
Vapor Density	4.00	(Air = 1.0)
Specific Gravity / Density	0.922	
Bulk Density	Not applicable	Liquid
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C6 H12 O2	
Molecular Weight	116.15	

## SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Incompatible products. Excess heat.
Materials to avoid	Strong oxidizing agents. Strong bases.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Isohexanoic acid	2050 mg/kg ( Rat )	968 mg/kg ( Rabbit )	

(b) skin corrosion/irritation; Category 1 C

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;  
Respiratory No data available

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<b>Skin</b>	No data available
<b>(e) germ cell mutagenicity;</b>	No data available
<b>(f) carcinogenicity;</b>	No data available There are no known carcinogenic chemicals in this product
<b>(g) reproductive toxicity;</b>	No data available
<b>(h) STOT-single exposure;</b>	No data available
<b>(i) STOT-repeated exposure;</b>	No data available
<b>Target Organs</b>	No information available.
<b>(j) aspiration hazard;</b>	No data available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.
<b>Symptoms / effects, both acute and delayed</b>	Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

**SECTION 12. ECOLOGICAL INFORMATION**

<b>Ecotoxicity effects</b>	Do not empty into drains.
<b>Persistence and Degradability Persistence</b>	Insoluble in water, May persist, based on information available.
<b>Bioaccumulative Potential</b>	May have some potential to bioaccumulate
<b>Mobility in soil</b>	Spillage unlikely to penetrate soil The product is insoluble and floats on water The product evaporates slowly Is not likely mobile in the environment due its low water solubility Spillage unlikely to penetrate soil
<b>Endocrine Disruptor Information Persistent Organic Pollutant Ozone Depletion Potential</b>	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance

**SECTION 13. DISPOSAL CONSIDERATIONS**

<b>Waste from Residues/Unused Products</b>	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
<b>Contaminated Packaging</b>	Dispose of this container to hazardous or special waste collection point.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

## SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No UN2922  
Proper Shipping Name Corrosive liquid, toxic, n.o.s.  
Hazard Class 8  
Subsidiary Hazard Class 6.1  
Packing Group III

IMDG/IMO

UN-No UN2922  
Proper Shipping Name Corrosive liquid, toxic, n.o.s.  
Hazard Class 8  
Subsidiary Hazard Class 6.1  
Packing Group III

IATA

UN-No UN2922  
Proper Shipping Name Corrosive liquid, toxic, n.o.s.  
Hazard Class 8  
Subsidiary Hazard Class 6.1  
Packing Group III

Special Precautions for User No special precautions required

## SECTION 15. REGULATORY INFORMATION

**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Isohexanoic acid	-	-	X	X	211-464-0	X	X	X	X	X	X	KE-25414

**National Regulations**

## SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department  
Creation Date 07-Mar-2012  
Revision Date 16-May-2024  
Revision Summary New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

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Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

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**End of Safety Data Sheet**