

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

### 1.1. Product identifier

**Product Description:** 4-Methylvaleric acid  
**Cat No. :** 255510000; 255510050; 255510250  
**Synonyms** 4-Methylpentanoic acid; Isocaproic acid  
**CAS No** 646-07-1  
**EC No** 211-464-0  
**Molecular Formula** C6 H12 O2

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

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

### 1.3. Details of the supplier of the safety data sheet

#### Company

**UK entity/business name**  
 Fisher Scientific UK  
 Bishop Meadow Road,  
 Loughborough, Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
 Thermo Fisher Scientific  
 Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

**E-mail address** [begel.sdsdesk@thermofisher.com](mailto:begel.sdsdesk@thermofisher.com)

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

#### Physical hazards

Based on available data, the classification criteria are not met

#### Health hazards

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

Acute dermal toxicity  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation

Category 3 (H311)  
Category 1 C (H314)  
Category 1 (H318)

### **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

### **Hazard Statements**

H314 - Causes severe skin burns and eye damage  
H311 - Toxic in contact with skin

### **Precautionary Statements**

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

## **2.3. Other hazards**

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

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Isohexanoic acid	646-07-1	EEC No. 211-464-0	>95	Skin Corr. 1C (H314) Eye Dam. 1 (H318) Acute Tox. 3 (H311)

Full text of Hazard Statements: see section 16

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>General Advice</b>	Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.
<b>Eye Contact</b>	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.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Inhalation</b>	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.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

### 4.2. Most important symptoms and effects, both acute and delayed

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

### 4.3. Indication of any immediate medical attention and special treatment needed

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### 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.

### 5.2. Special hazards arising from the substance or mixture

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

#### Hazardous Combustion Products

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

### 5.3. Advice 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

ACR25551

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## 6.1. Personal precautions, protective equipment and emergency procedures

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

## 6.2. Environmental precautions

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

## 6.3. Methods and material for containment and cleaning up

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

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe 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.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

### 7.2. Conditions for safe storage, including any incompatibilities

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 6.1C  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

List source(s):

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. 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	See manufacturers	-	EN 374	(minimum requirement)
Butyl rubber	recommendations			
Nitrile rubber				
Neoprene				
PVC				

**Skin and body protection** Long sleeved clothing.

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 compatibility, 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.

**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

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Clear	
<b>Odor</b>	pungent	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	-35 °C / -31 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	200 °C / 392 °F	@ 760 mmHg
<b>Flammability (liquid)</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	97 °C / 206.6 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No information available	
<b>Density / Specific Gravity</b>	0.922	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	4.00	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

## 9.2. Other information

<b>Molecular Formula</b>	C6 H12 O2
<b>Molecular Weight</b>	116.15

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Excess heat.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong bases.

### 10.6. 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

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

### Product Information

#### (a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

Category 3

Inhalation

Based on available data, the classification criteria are not met

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

Skin

No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs

No information available.

(j) aspiration hazard; No data available

#### Other Adverse Effects

The toxicological properties have not been fully investigated.

#### Symptoms / effects, both acute and delayed

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.

## 11.2. Information on other hazards

#### Endocrine Disrupting Properties

Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

**Ecotoxicity effects** Do not empty into drains.

## **12.2. Persistence and degradability**

**Persistence** Insoluble in water, May persist, based on information available.

**12.3. Bioaccumulative potential** May have some potential to bioaccumulate

## **12.4. Mobility in soil**

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

**12.5. Results of PBT and vPvB assessment** No data available for assessment.

## **12.6. Endocrine disrupting properties**

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

## **12.7. Other adverse effects**

**Persistent Organic Pollutant** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## **SECTION 13: DISPOSAL CONSIDERATIONS**

### **13.1. Waste treatment methods**

**Waste from Residues/Unused Products** 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.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point.

**European Waste Catalogue (EWC)** According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

**Other Information** 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**

### **IMDG/IMO**

**14.1. UN number** UN2922  
**14.2. UN proper shipping name** Corrosive liquid, toxic, n.o.s.  
**14.3. Transport hazard class(es)** 8  
**Subsidiary Hazard Class** 6.1  
**14.4. Packing group** III



# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

## ADR

**14.1. UN number** UN2922  
**14.2. UN proper shipping name** Corrosive liquid, toxic, n.o.s.  
**14.3. Transport hazard class(es)** 8  
**Subsidiary Hazard Class** 6.1  
**14.4. Packing group** III

## IATA

**14.1. UN number** UN2922  
**14.2. UN proper shipping name** Corrosive liquid, toxic, n.o.s.  
**14.3. Transport hazard class(es)** 8  
**Subsidiary Hazard Class** 6.1  
**14.4. Packing group** III

**14.5. Environmental hazards** No hazards identified  
**14.6. Special precautions for user** No special precautions required.  
**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Isohexanoic acid	646-07-1	211-464-0	-	-	X	X	KE-25414	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Isohexanoic acid	646-07-1	X	ACTIVE	X	-	X	X	X

**Legend:** X - Listed '-' - Not Listed      **KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**Authorisation/Restrictions according to EU REACH** Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Isohexanoic acid	646-07-1	-	-	-

#### Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Isohexanoic acid	646-07-1	Not applicable	Not applicable

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 3 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H311 - Toxic in contact with skin

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

### 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/NDSL - 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 Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

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

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

OECD - Organisation for Economic Co-operation and Development

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

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

# SAFETY DATA SHEET

4-Methylvaleric acid

Revision Date 29-Sep-2023

BCF - Bioconcentration factor

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

## Training Advice

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

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.

Creation Date	07-Mar-2012
Revision Date	29-Sep-2023
Revision Summary	Not applicable.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**