

Page 1/8 Creation Date 21-Oct-2010 Revision Date 30-Apr-2024 Version 3

ALFAAL06007

# Methyl 4,4-dimethyl-3-oxovalerate

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

产品说明: 甲基 4,4-二甲基-3-氧代戊酸甲酯 Product Description: Methyl 4,4-dimethyl-3-oxovalerate

Cat No. : L06007

**Synonyms** Pentanoic acid, 4,4-dimethyl-3-oxo, methyl ester

CAS No 55107-14-7 Molecular Formula C8 H14 O3

**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 Appearance Odor

Liquid Clear Colorless No information available

**Emergency Overview** 

Combustible liquid. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

### Classification of the substance or mixture

Flammable liquids.	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

#### **Label Elements**



Signal Word Warning

Page 2/8 Revision Date 30-Apr-2024

### Methyl 4,4-dimethyl-3-oxovalerate

#### **Hazard Statements**

H227 - Combustible liquid

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

### **Precautionary Statements**

#### Prevention

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

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

P271 - Use only outdoors or in a well-ventilated area

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

#### Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

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

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

P312 - Call a POISON CENTER or doctor if you feel unwell

P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

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

#### Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

#### **Disposal**

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

#### **Physical and Chemical Hazards**

Combustible material.

#### **Health Hazards**

Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

#### **Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

#### Other Hazards

This product does not contain any known or suspected endocrine disruptors.

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

Component	CAS No	Weight %
Pentanoic acid, 4,4-dimethyl-3-oxo-, methyl ester	55107-14-7	>95

### **SECTION 4. FIRST AID MEASURES**

#### **General Advice**

If symptoms persist, call a physician.

#### Eve Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

#### **Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

#### Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

### Ingestion

Page 3/8 Revision Date 30-Apr-2024

Methyl 4,4-dimethyl-3-oxovalerate

Clean mouth with water and drink afterwards plenty of water.

#### Most important symptoms and effects

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

#### Self-Protection of the First Aider

Use personal protective equipment as required.

#### **Notes to Physician**

Treat symptomatically.

### **SECTION 5. FIRE-FIGHTING MEASURES**

#### **Suitable Extinguishing Media**

Use:. Dry chemical. Carbon dioxide (CO<sub>2</sub>). Water spray. Alcohol resistant foam. Water mist may be used to cool closed containers.

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

No information available.

### **Specific Hazards Arising from the Chemical**

Keep product and empty container away from heat and sources of ignition. Risk of ignition. Combustible material. Containers may explode when heated.

### **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.

### **SECTION 6. ACCIDENTAL RELEASE MEASURES**

## **Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

#### **Environmental Precautions**

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

### Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

### **SECTION 7. HANDLING AND STORAGE**

### Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition.

### Storage

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

### Specific Use(s)

Use in laboratories

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

### **Control Parameters**

Page 4/8 Revision Date 30-Apr-2024

Methyl 4,4-dimethyl-3-oxovalerate

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#### 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 MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

#### **Exposure Controls**

#### **Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. 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 Natural rubber Butyl rubber Nitrile rubber	Breakthrough time See manufacturers recommendations	Glove thickness	<b>EU standard</b> EN 374	Glove comments (minimum requirement)
Neoprene PVC				

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** No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use Maintain adequate ventilation

Hygiene Measures When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area

and clothing.

**Environmental exposure controls** No information available.

### **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Appearance Clear Colorless

Physical State Liquid

Odor No information available
Odor Threshold No data available
pH No information available

Page 5/8 Revision Date 30-Apr-2024

### Methyl 4,4-dimethyl-3-oxovalerate

Liquid

(Air = 1.0)

explosive air/vapour mixtures possible

Melting Point/RangeNo data availableSoftening PointNo data available

**Boiling Point/Range** 67 - 70 °C / 152.6 - 158 °F @ 13 mmHg

Flash Point 78 °C / 172.4 °F Method - No information available

Evaporation Rate No data available Flammability (solid,gas) Not applicable

Explosion Limits No data available

Vapor Pressure 0.4 kPa @ 20 mmHg

Vapor Density No data available

Specific Gravity / Density 0.98

Bulk Density Not applicable Liquid

Water Solubility

Solubility

No information available
No information available

Partition Coefficient (n-octanol/water)

Autoignition Temperature

Decomposition Temperature

Viscosity

No data available

No data available

No data available

**Explosive Properties** 

Oxidizing Properties No information available

Molecular FormulaC8 H14 O3Molecular Weight158.20

## **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. Keep away from open flames, hot surfaces and

sources of ignition.

Materials to avoid Strong oxidizing agents.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO2).

# **SECTION 11. TOXICOLOGICAL INFORMATION**

Product Information No acute toxicity information is available for this product

(a) acute toxicity;

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(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

Page 6/8 Revision Date 30-Apr-2024

Methyl 4,4-dimethyl-3-oxovalerate

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system

(i) STOT-repeated exposure; No data available

No information available. **Target Organs** 

No data available (j) aspiration hazard;

Symptoms / effects, both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

delayed

### **SECTION 12. ECOLOGICAL INFORMATION**

**Ecotoxicity effects** 

Persistence and Degradability

No information available **Persistence** 

Persistence is unlikely, based on information available.

**Bioaccumulative Potential** Bioaccumulation is unlikely

The product contains volatile organic compounds (VOC) which will evaporate easily from all Mobility in soil

surfaces Will likely be mobile in the environment due to its volatility Disperses rapidly in air

**Endocrine Disruptor Information** 

**Persistent Organic Pollutant Ozone Depletion Potential** 

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**

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.

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

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.

### **SECTION 14. TRANSPORT INFORMATION**

**Road and Rail Transport** Not Regulated

Not regulated IMDG/IMO

**Page** 7/8 Revision Date 30-Apr-2024

Methyl 4,4-dimethyl-3-oxovalerate

IATA Not regulated

**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)	goods GB	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Pentanoic acid, 4,4-dimethyl-3-oxo-, methyl ester	-	-	X	X	259-481-2	Х	-	X	X	Х	-	-

### **National Regulations**

### **SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department

**Creation Date** 21-Oct-2010 30-Apr-2024 **Revision Date** 

**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.

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

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

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances IECSC - Chinese Inventory of Existing Chemical Substances

AICS - Australian Inventory of Chemical Substances **KECL** - Korean Existing and Evaluated 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%

Substances List

EC50 - Effective Concentration 50% POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ALFAAL06007

# SAFETY DATA SHEET

Page 8 / 8 Revision Date 30-Apr-2024

### Methyl 4,4-dimethyl-3-oxovalerate

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

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**