

ALFAAA10991

Methyl octanoate

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

产品说明: Product Description:	辛酸甲酯 Methyl octanoate
Cat No. :	A10991
Synonyms	Methyl caprylate
CAS No	111-11-5
Molecular Formula	C9 H18 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 Colorless	Odor sweet
Emergency Overview Combustible liquid.		

Classification of the substance or mixture

Flammable liquids.	Category 4
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Label Elements

None required

Signal Word **Warning**

Hazard Statements
H227 - Combustible liquid

Precautionary Statements
Prevention

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

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

Storage

P403 + P235 - Store in a well-ventilated place. Keep cool

Disposal

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

Physical and Chemical Hazards

Combustible material.

Health Hazards

The product contains no substances which at their given concentration are considered to be hazardous to health.

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 %
Methyl ester octanoic acid	111-11-5	>95

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

If symptoms persist, call a physician. 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. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.

Inhalation

Remove to fresh air. Get medical attention immediately if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Most important symptoms and effects

None reasonably foreseeable. . Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

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

Water spray, carbon dioxide (CO2), dry chemical, 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**

Use personal protective equipment as required. Ensure adequate ventilation. 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

Sweep up and shovel into suitable 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. Avoid contact with skin, eyes or 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****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**

None under normal use conditions. Ensure adequate ventilation, especially in confined areas. .

Personal protective equipment**Eye Protection**

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

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Hand Protection

Protective gloves

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

Wear appropriate protective gloves and clothing to prevent skin exposure Chemical resistant apron Antistatic boots Impervious gloves

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

Recommended Filter type: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

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

Colorless

Physical State

Liquid

Odor

sweet

Odor Threshold

No data available

pH

No information available

Melting Point/Range

No data available

Softening Point

No data available

Boiling Point/Range

79 °C / 174.2 °F

Flash Point

73 °C / 163.4 °F

@ 12 mm Hg

Method - No information available

Evaporation Rate

No data available

Flammability (solid,gas)

Not applicable

Liquid

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

5.46

(Air = 1.0)

Specific Gravity / Density

0.878

Bulk Density

Not applicable

Liquid

Water Solubility

Insoluble

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

Component

log Pow

Methyl ester octanoic acid

3.32

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Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	

Molecular Formula	C9 H18 O2
Molecular Weight	158.24

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	Oxidizing agent.

Hazardous Decomposition Products 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
Methyl ester octanoic acid	>2000 mg/kg (Rat)		

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(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. See actual entry in RTECS for complete information

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability
Persistence Persistence is unlikely, based on information available.

Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
Methyl ester octanoic acid	3.32	No data available

Mobility in soil The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

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

Waste from Residues/Unused Products Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Contaminated Packaging Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

Other Information Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport Not Regulated

IMDG/IMO Not regulated

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)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Methyl ester octanoic acid	-	-	X	X	203-835-0	X	X	X	X	X	X	KE-24532

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 10-Feb-2011
Revision Date 27-Apr-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.

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

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