ALFAAB21242

Methyl 2-octynoate

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

产品说明: 2-辛酸甲酯
Product Description: **Methyl 2-octynoate**

Cat No. : **B21242**
CAS No 111-12-6
Molecular Formula CH3 (CH2)4 C#CCO2 CH3

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	No information available	No information available

Emergency Overview

Combustible liquid. May be harmful in contact with skin. May cause an allergic skin reaction. Very toxic to aquatic life. Harmful to aquatic life with long lasting effects. Lachrymator (substance which increases the flow of tears).

Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Dermal Toxicity	Category 5
Skin Sensitization	Category 1
Acute aquatic toxicity	Category 1
Chronic aquatic toxicity	Category 3

Label Elements

Signal Word **Warning**

Hazard Statements
H227 - Combustible liquid
H313 - May be harmful in contact with skin
H317 - May cause an allergic skin reaction
H400 - Very toxic to aquatic life
H412 - Harmful to aquatic life with long lasting effects

Precautionary Statements
Prevention
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P272 - Contaminated work clothing should not be allowed out of the workplace
P280 - Wear protective gloves/protective clothing/eye protection/face protection
Response
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention
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 + 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
May be harmful in contact with skin. May cause an allergic skin reaction. Lachrymator (substance which increases the flow of tears).
Environmental hazards
Very toxic to aquatic life. Harmful to aquatic life with long lasting effects.

Other Hazards
Lachrymator (substance which increases the flow of tears)
This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Methyl heptine carbonate	111-12-6	<=100

SECTION 4. FIRST AID MEASURES

General Advice
If symptoms persist, call a physician.

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. 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
Clean mouth with water and drink afterwards plenty of water.

Most important symptoms and effects

Difficulty in breathing. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

Self-Protection of the First Aider
No special precautions required.

Notes to Physician
Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media
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
Combustible material. Containers may explode when heated. Do not allow run-off from fire-fighting to enter drains or water courses.

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
Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

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. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. 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

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)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber Neoprene Natural rubber 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 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 Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance
Physical State Liquid

Odor No information available
Odor Threshold No data available
pH No information available
Melting Point/Range No data available
Softening Point No data available
Boiling Point/Range 216 - 218 °C / 420.8 - 424.4 °F
Flash Point 88 °C / 190.4 °F **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	No data available	(Air = 1.0)
Specific Gravity / Density	0.92 g/cm3	@ 20 °C
Bulk Density	Not applicable	Liquid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	**log Pow**	
Methyl heptine carbonate	3	
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	CH3 (CH2)4 C#CCO2 CH3	
Molecular Weight	154.20	

SECTION 10. STABILITY AND REACTIVITY

Stability Stable under normal conditions.

Hazardous Reactions None under normal processing.
Hazardous Polymerization No information available.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition.

Materials to avoid No information available.

Hazardous Decomposition Products None under normal use conditions.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Methyl heptine carbonate	LD50 = 1530 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 Category 1

May cause sensitization by skin contact

(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

Symptoms / effects,both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects The product contains following substances which are hazardous for the environment. Very toxic to aquatic organisms.

Persistence and Degradability No information available
Degradation in sewage treatment plant Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential No information available

Component	log Pow	Bioconcentration factor (BCF)
Methyl heptine carbonate	3	No data available

Mobility in soil No information available

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 Should not be released into the environment. 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.

Other Information Do not flush to sewer. 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 let this chemical enter the environment.

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	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Methyl heptine carbonate	-	-	X	203-836-6	X	X	X	X	X	X	KE-24561

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 27-Jul-2026
Revision Summary Not applicable.

Training Advice
Chemical incident response training.

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