

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

### 1.1. Product identifier

Product Description:	<b>Methyl octanoate</b>
Cat No. :	<b>A10991</b>
Synonyms	Methyl caprylate
CAS No	111-11-5
EC No	203-835-0
Molecular Formula	C9 H18 O2
REACH registration number	-

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

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Based on available data, the classification criteria are not met

**Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements

### Hazard Statements

Combustible liquid

### Precautionary Statements

## 2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

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
Methyl ester octanoic acid	111-11-5	EEC No. 203-835-0	>95	-

REACH registration number

-

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of 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

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immediately if symptoms occur.

## Ingestion

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

## Inhalation

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

## Self-Protection of the First Aider

No special precautions required.

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

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

### 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. Water mist may be used to cool closed containers.

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

No information available.

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

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

#### Hazardous Combustion Products

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.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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

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

### 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

Sweep up and shovel into suitable containers for disposal. Remove all sources of ignition.

### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

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## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe 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.

### Hygiene Measures

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

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

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 10  
**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

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

#### 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

#### Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
Methyl ester octanoic acid 111-11-5 ( >95 )	PNEC = 0.0018mg/L	PNEC = 0.0276mg/kg sediment dw	PNEC = 0.0476mg/L	PNEC = 100mg/L	PNEC = 10mg/kg soil dw

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Methyl ester octanoic acid 111-11-5 ( >95 )	PNEC = 0.00018mg/L	PNEC = 0.0028mg/kg sediment dw		PNEC = 66.6mg/kg food	

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

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure. Chemical resistant apron. Antistatic boots. Impervious gloves.

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** 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

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Liquid	
<b>Appearance</b>	Colorless	
<b>Odor</b>	sweet	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	79 °C / 174.2 °F	@ 12 mm Hg
<b>Flammability (liquid)</b>	Combustible liquid	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	73 °C / 163.4 °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	

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## Partition Coefficient (n-octanol/water)

<b>Component</b>	<b>log Pow</b>	
Methyl ester octanoic acid	3.32	
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	0.878	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	5.46	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

## 9.2. Other information

<b>Molecular Formula</b>	C9 H18 O2
<b>Molecular Weight</b>	158.24
<b>Explosive Properties</b>	explosive air/vapour mixtures possible

## 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. Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

Oxidizing agent.

### 10.6. Hazardous decomposition products

Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

#### (a) acute toxicity;

<b>Oral</b>	Based on available data, the classification criteria are not met
<b>Dermal</b>	No data available
<b>Inhalation</b>	No data available

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;

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<b>Respiratory</b>	No data available
<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. See actual entry in RTECS for complete information
<b>Symptoms / effects, both acute and delayed</b>	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 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

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

### 12.2. Persistence and degradability

**Persistence** Persistence is unlikely, based on information available.

### 12.3. Bioaccumulative potential

Bioaccumulation is unlikely

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

### 12.4. 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

### 12.5. Results of PBT and vPvB assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

### 12.6. Endocrine disrupting

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## 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** 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.

**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.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO** Not regulated

### 14.1. UN number

### 14.2. UN proper shipping name

### 14.3. Transport hazard class(es)

### 14.4. Packing group

**ADR** Not regulated

### 14.1. UN number

### 14.2. UN proper shipping name

### 14.3. Transport hazard class(es)

### 14.4. Packing group

**IATA** Not regulated

### 14.1. UN number

### 14.2. UN proper shipping name

### 14.3. Transport hazard class(es)

### 14.4. Packing group

**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



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## 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
Methyl ester octanoic acid	111-11-5	203-835-0	-	-	X	X	KE-24532	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Methyl ester octanoic acid	111-11-5	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)
Methyl ester octanoic acid	111-11-5	-	-	-

### 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
Methyl ester octanoic acid	111-11-5	Not applicable	Not applicable

### 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

See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Methyl ester octanoic acid	WGK1	

## 15.2. Chemical safety assessment

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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

#### 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/MDG** - International Maritime Organization/International Maritime Dangerous Goods Code

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

**BCF** - Bioconcentration factor

#### Key literature references and sources for data

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

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

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

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

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

#### Training Advice

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

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

**Creation Date** 10-Feb-2011

**Revision Date** 05-Feb-2024

**Revision Summary** New emergency telephone response service provider.

**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**