

SAFETY DATA SHEET

Creation Date 10-Feb-2011

Revision Date 28-Mar-2024

Revision Number 4

1. Identification

Product Name Methyl octanoate

Cat No. : L05740

CAS No 111-11-5
Synonyms Methyl caprylate

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

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

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids

Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid

Precautionary Statements

Prevention

Keep away from heat/sparks/open flames/hot surfaces. - No smoking

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

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep cool

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Methyl ester octanoic acid	111-11-5	>95

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
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	Do not use a solid water stream as it may scatter and spread fire
Flash Point	73 °C / 163.4 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	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.

Hazardous Combustion Products

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

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.

NFPA

Health
0

Flammability
2

Instability
0

Physical hazards
N/A

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.

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. Incompatible Materials. Oxidizing agent.

8. Exposure controls / personal protection**Exposure Guidelines**

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

Engineering Measures

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

Personal Protective Equipment**Eye/face Protection**

Tight sealing safety goggles.

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.

Recommended Filter type:

Particle filter.

Hygiene Measures

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

9. Physical and chemical properties**Physical State**

Liquid

Appearance

Colorless

Odor

sweet

Odor Threshold

No information available

pH

No information available

Melting Point/Range	No data available
Boiling Point/Range	79 °C / 174.2 °F @ 12 mm Hg
Flash Point	73 °C / 163.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	5.46
Specific Gravity	0.878
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C9 H18 O2
Molecular Weight	158.24

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Oxidizing agent
Hazardous Decomposition Products	Thermal decomposition can lead to release of irritating gases and vapors
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Methyl ester octanoic acid	>2000 mg/kg (Rat)	Not listed	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Methyl ester octanoic acid	111-11-5	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	None known
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

Component	log Pow
Methyl ester octanoic acid	3.32

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk.

UN-No NA1993
Proper Shipping Name Combustible liquid, n.o.s.
Packing Group III

TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Methyl ester octanoic acid	111-11-5	X	ACTIVE	TP

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TP - Indicates a substance that is the subject of a proposed TSCA Section 4 test rule

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Methyl ester octanoic acid	111-11-5	X	-	203-835-0	X	X	X	X	X	KE-24532

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

Not applicable

Clean Air Act

Not applicable

OSHA - Occupational Safety and Health Administration

Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security

This product does not contain any DHS chemicals.

Other International Regulations**Mexico - Grade**

Moderate risk, Grade 2

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	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Methyl ester octanoic acid	111-11-5	Listed	Not applicable	Not applicable	Not applicable

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

Not applicable

Other International Regulations

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Methyl ester octanoic acid	111-11-5	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

Health, Safety and Environmental Department
Email: chem.techinfo@thermofisher.com
www.thermofisher.com

Creation Date

10-Feb-2011

Revision Date

28-Mar-2024

Print Date

28-Mar-2024

Revision Summary

New emergency telephone response service provider.

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 SDS