

1. Identification

Product identifier	METHYL OCTINE CARBONATE	
Other means of identification		
BRI Product Code	485	
CAS number	111-80-8	
FEMA number	2726	
Synonyms	2-Nonynoic acid, methyl ester * Methyl 2-nonynoate * MOC	
Recommended use	flavors and fragrances For Manufacturing Use Only	
Recommended restrictions	Not for use in Tobacco or Nicotine delivery device applications and/or products.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	Bedoukian Research	
Address	6 Commerce Drive Danbury, CT 06810 United States	
Telephone	1-203-830-4000	
Website	www.bedoukian.com	
E-mail	customerservice@bedoukian.com	
Contact person	Joseph Bania	
Emergency phone number	Chemtrec (North America)	1-800-424-9300
	Chemtrec (International)	1-703-527-3887

2. Hazard(s) identification

Physical hazards	Not classified.	
Health hazards	Acute toxicity, oral	Category 4
	Sensitization, skin	Category 1
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Warning	
Hazard statement	Harmful if swallowed. May cause an allergic skin reaction.	
Precautionary statement		
Prevention	Avoid breathing mist or vapor. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Contaminated work clothing must not be allowed out of the workplace. Wear protective gloves.	
Response	If swallowed: Call a poison center/doctor if you feel unwell. Rinse mouth. If on skin: Wash with plenty of water. If skin irritation or rash occurs: Get medical advice/attention. Wash contaminated clothing before reuse.	
Storage	Store away from incompatible materials.	
Disposal	Dispose of contents/container in accordance with relevant area regulations.	
Hazard(s) not otherwise classified (HNOC)	None known.	
Supplemental information	None.	

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
METHYL OCTINE CARBONATE	2-Nonynoic acid, methyl ester Methyl 2-nonynoate MOC	111-80-8	100

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.1

*Designates that a specific chemical identity and/or percentage of composition has been withheld as a trade secret.

Composition comments Occupational Exposure Limits for stabilizers are listed in Section 8.

4. First-aid measures

Inhalation	Move to fresh air. Call a physician if symptoms develop or persist.
Skin contact	Remove contaminated clothing immediately and wash skin with soap and water. In case of eczema or other skin disorders: Seek medical attention and take along these instructions.
Eye contact	Rinse with water. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Get medical advice/attention if you feel unwell.
Most important symptoms/effects, acute and delayed	May cause an allergic skin reaction. Dermatitis. Rash.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically. Keep victim warm. Keep victim under observation. Symptoms may be delayed.
General information	Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. Show this safety data sheet to the doctor in attendance. Wash contaminated clothing before reuse.

5. Fire-fighting measures

Suitable extinguishing media	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO2).
Unsuitable extinguishing media	Do not use water jet as an extinguisher, as this will spread the fire.
Specific hazards arising from the chemical	During fire, gases hazardous to health may be formed.
Special protective equipment and precautions for firefighters	Self-contained breathing apparatus and full protective clothing must be worn in case of fire.
Fire fighting equipment/instructions	Move containers from fire area if you can do so without risk.
Specific methods	Use standard firefighting procedures and consider the hazards of other involved materials.
General fire hazards	No unusual fire or explosion hazards noted.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Wear appropriate protective equipment and clothing during clean-up. Avoid breathing mist or vapor. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Absorb in vermiculite, dry sand or earth and place into containers. Following product recovery, flush area with water. Small Spills: Wipe up with absorbent material (e.g. cloth, fleece). Clean surface thoroughly to remove residual contamination.
Environmental precautions	Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS. Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	Do not taste or swallow. Avoid breathing mist or vapor. Avoid contact with eyes, skin, and clothing. When using, do not eat, drink or smoke. Provide adequate ventilation. Wear appropriate personal protective equipment. Wash hands thoroughly after handling. Observe good industrial hygiene practices.
Conditions for safe storage, including any incompatibilities	Store in original tightly closed container. Store away from incompatible materials (see Section 10 of the SDS). Recommended Packaging: Glass, Plastic, Aluminum or Phenolic Lined Steel. Store tightly sealed under inert gas in a cool, well-ventilated area.

8. Exposure controls/personal protection

Occupational exposure limits	This substance has no PEL, TLV, or other recommended exposure limit.
Biological limit values	No biological exposure limits noted for the ingredient(s).
Appropriate engineering controls	Good general ventilation (typically 10 air changes per hour) should be used. Ventilation rates should be matched to conditions. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level.
Individual protection measures, such as personal protective equipment	
Eye/face protection	Face shield is recommended. Wear safety glasses with side shields (or goggles).
Skin protection	
Hand protection	Wear appropriate chemical resistant gloves.
Other	Wear appropriate chemical resistant clothing. Use of an impervious apron is recommended.
Respiratory protection	In case of insufficient ventilation, wear suitable respiratory equipment.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	Keep away from food and drink. Always observe good personal hygiene measures, such as washing after handling the material and before eating, drinking, and/or smoking. Routinely wash work clothing and protective equipment to remove contaminants. Contaminated work clothing should not be allowed out of the workplace.

9. Physical and chemical properties

Appearance	
Physical state	Liquid.
Color	colorless to pale yellow
Odor	green, violet-leaf odor.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	436.15 °F (224.53 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Flash point	220 °F (104 °C) Closed Cup
Evaporation rate	Not available.
Flammability (solid, gas)	Not applicable.
Upper/lower flammability or explosive limits	
Flammability limit - lower (%)	Not available.
Flammability limit - upper (%)	Not available.
Explosive limit - lower (%)	Not available.
Explosive limit - upper (%)	Not available.
Vapor pressure	0.06 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	5.8 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.

Partition coefficient (n-octanol/water)	3.1 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Density	0.911 - 0.918 g/cm ³
Explosive properties	Not explosive.
Flammability class	Combustible IIIB estimated
Molecular formula	C ₁₀ H ₁₆ O ₂
Molecular weight	168.24
Oxidizing properties	Not oxidizing.
Specific gravity	0.911 - 0.918 at 25°C

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	No hazardous decomposition products are known.

11. Toxicological information

Information on likely routes of exposure

Inhalation	No adverse effects due to inhalation are expected.
Skin contact	May cause an allergic skin reaction.
Eye contact	Direct contact with eyes may cause temporary irritation.
Ingestion	Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics May cause an allergic skin reaction. Dermatitis. Rash.

Information on toxicological effects

Acute toxicity Harmful if swallowed.

Product	Species	Test Results
METHYL OCTINE CARBONATE (CAS 111-80-8)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	3000 - 5000 mg/kg
Oral		
<i>Liquid</i>		
LD50	Rat	1600 mg/kg

* Estimates for product may be based on additional component data not shown.

Skin corrosion/irritation Prolonged skin contact may cause temporary irritation.

Irritation Corrosion - Skin

METHYL OCTINE CARBONATE

2.5 - 100 % Patch test, Vehicle 80% Ethanol/20% distilled water. Slight to moderate erythema.
Result: Irritation noted.
Species: Guinea pig
Organ: Skin
Notes: RIFM

Serious eye damage/eye irritation Direct contact with eyes may cause temporary irritation.

Irritation Corrosion - Eye

METHYL OCTINE CARBONATE

100 %
Result: Not irritating.
Species: Rabbit
Organ: Eye
Notes: RIFM

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization May cause an allergic skin reaction.

Skin sensitization

METHYL OCTINE CARBONATE

2 % Patch test, Vehicle was 75% Ethanol, 25% Diethyl phthalate. Strong reaction displayed in 45/106 panelists.
Result: Sensitization noted.
Species: Human
Organ: Skin
Notes: RIFM
LLNA
Result: Sensitization noted.
Species: Mouse
Notes: ECHA

Germ cell mutagenicity No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.

Germ cell mutagenicity: Ames test

METHYL OCTINE CARBONATE

< 3600 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100 with and without metabolic activation. Vehicle DMSO or water.
Result: Not mutagenic.
Species: Salmonella typhimurium
Notes: RIFM

Carcinogenicity Not classifiable as to carcinogenicity to humans.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity This product is not expected to cause reproductive or developmental effects.

Specific target organ toxicity - single exposure Not classified.

Specific target organ toxicity - repeated exposure Not classified.

Aspiration hazard Not an aspiration hazard.

12. Ecological information

Ecotoxicity The product is not classified as environmentally hazardous. However, this does not exclude the possibility that large or frequent spills can have a harmful or damaging effect on the environment.

Persistence and degradability No data is available on the degradability of this product.

Biodegradability

Percent degradation (Aerobic biodegradation-inherent)

METHYL OCTINE CARBONATE

71 % OECD 301F, 30 mg/L.
Result: Inherently biodegradable.
Species: Activated sludge of a predominantly domestic sewage
Test Duration: 28 days

Percent degradation (Aerobic biodegradation-ready)

METHYL OCTINE CARBONATE

61 % OECD 301F, 30 mg/L. 10-day criteria fulfilled.
Result: Readily biodegradable.
Species: Activated sludge of a predominantly domestic sewage
Test Duration: 10 days

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)
METHYL OCTINE CARBONATE

3.1, US EPA. 2014. Estimation Programs Interface Suite™
for Microsoft® Windows, v 4.11. US EPA, Washington, DC,
USA.

Mobility in soil

No data available.

Other adverse effects

No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations

Disposal instructions

Collect and reclaim or dispose in sealed containers at licensed waste disposal site. Dispose of contents/container in accordance with local/regional/national/international regulations.

Local disposal regulations

Dispose in accordance with all applicable regulations.

Hazardous waste code

The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products

Dispose of in accordance with local regulations. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Since emptied containers may retain product residue, follow label warnings even after container is emptied. Empty containers should be taken to an approved waste handling site for recycling or disposal.

14. Transport information

DOT

Not regulated as dangerous goods.

IATA

Not regulated as dangerous goods.

IMDG

Not regulated as dangerous goods.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not established.

15. Regulatory information

US federal regulations

This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not regulated.

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Hazard categories

Immediate Hazard - Yes
Delayed Hazard - No
Fire Hazard - No
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical Yes

SARA 313 (TRI reporting)

Not regulated.

Other federal regulations

Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.

US state regulations

California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins.

International Inventories

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
Taiwan	Taiwan Toxic Chemical Substances (TCS)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

IFRA restriction

There is an IFRA guideline regarding this product. Please visit www.ifra.org for the full text of the guideline, or contact Bedoukian Research, Inc. for more information.

16. Other information, including date of preparation or last revision

Issue date 17-May-2015

Revision date 02-July-2020

Version # 02

Disclaimer

Bedoukian Research cannot anticipate all conditions under which this information and its product, or the products of other manufacturers in combination with its product, may be used. It is the user's responsibility to ensure safe conditions for handling, storage and disposal of the product, and to assume liability for loss, injury, damage or expense due to improper use. The information in the sheet was written based on the best knowledge and experience currently available.

Revision information

This document has undergone significant changes and should be reviewed in its entirety.