

1. Identification

Product identifier	GUAVANATE™	
Other means of identification		
BRI Product Code	493	
CAS number	41654-15-3	
FEMA number	4165	
Synonyms	5-Octenoic acid, methyl ester, (5Z)- * METHYL CIS-5-OCTENOATE * Methyl z-5-octenoate	
Recommended use	flavors and fragrances For Manufacturing Use Only	
Recommended restrictions	BRI's Products are not for use in tobacco products, e cigarettes, or any other nicotine delivery devices; nor for use in non-tobacco delivery mechanisms such as vaping devices.	
Manufacturer/Importer/Supplier/Distributor information		
Manufacturer		
Company name	Bedoukian Research Inc (BRI)	
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	Flammable liquids	Category 4
Health hazards	Serious eye damage/eye irritation	Category 2B
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		
Hazard symbol	None.	
Signal word	Warning	
Hazard statement	Combustible liquid. Causes eye irritation.	
Precautionary statement		
Prevention	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Wash thoroughly after handling. Wear protective gloves/eye protection/face protection.	
Response	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention. In case of fire: Use appropriate media to extinguish.	
Storage	Store in a well-ventilated place. Keep cool.	
Disposal	Dispose of contents/container in accordance with relevant area regulations.	
Hazard(s) not otherwise classified (HNOC)	None known.	
Supplemental information	100% of the mixture consists of component(s) of unknown acute hazards to the aquatic environment. 100% of the mixture consists of component(s) of unknown long-term hazards to the aquatic environment.	

3. Composition/information on ingredients

Substances

Chemical name	Common name and synonyms	CAS number	%
GUAVANATE™	5-Octenoic acid, methyl ester, (5Z)- METHYL CIS-5-OCTENOATE Methyl z-5-octenoate	41654-15-3	100

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

4. First-aid measures

Inhalation	Move to fresh air. Call a physician if symptoms develop or persist.
Skin contact	Wash off with soap and water. Get medical attention if irritation develops and persists.
Eye contact	Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Irritation of eyes. Exposed individuals may experience eye tearing, redness, and discomfort.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically. 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.

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	The product is combustible, and heating may generate vapors which may form explosive vapor/air mixtures. 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	In case of fire and/or explosion do not breathe fumes. 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	Combustible liquid.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Wear appropriate protective equipment and clothing during clean-up. 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	Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Keep combustibles (wood, paper, oil, etc.) away from spilled material. Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. Use a non-combustible material like vermiculite, sand or earth to soak up the product and place into a container for later disposal. Following product recovery, flush area with water. Small Spills: Absorb with earth, sand or other non-combustible material and transfer to containers for later disposal. Wipe up with absorbent material (e.g. cloth, fleece). Clean surface thoroughly to remove residual contamination. Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	Keep away from open flames, hot surfaces and sources of ignition. When using do not smoke. Avoid contact with eyes. Provide adequate ventilation. Wear appropriate personal protective equipment. Observe good industrial hygiene practices.
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Conditions for safe storage, including any incompatibilities

Keep away from heat, sparks and open flame. Store in a cool, dry place out of direct sunlight. Store in original tightly closed container. Store in a well-ventilated place. Keep in an area equipped with sprinklers. 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. Provide eyewash station.

Individual protection measures, such as personal protective equipment**Eye/face protection**

Wear safety glasses with side shields (or goggles).

Skin protection**Hand protection**

Wear appropriate chemical resistant gloves.

Other

Wear suitable protective clothing.

Respiratory protection

If engineering controls do not maintain airborne concentrations below recommended exposure limits (where applicable) or to an acceptable level (in countries where exposure limits have not been established), an approved respirator must be worn.

Thermal hazards

Wear appropriate thermal protective clothing, when necessary.

General hygiene considerations

When using do not smoke. 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.

9. Physical and chemical properties**Appearance****Physical state**

Liquid.

Color

Colorless

Odor

Fruity.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

203 °F (95 °C) at 25 mm Hg. Bedoukian obtained value.

386.69 °F (197.05 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Flash point

159 °F (71 °C) Closed Cup Bedoukian obtained value.

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

0.28 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Vapor density

5.4 Relative to air; air = 1

Relative density

Not available.

Solubility(ies)**Solubility (water)**

Not available.

Partition coefficient (n-octanol/water)	3.105 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	0.896 - 0.902 g/cm ³ at 25°C. Bedoukian obtained value.
Explosive properties	Not explosive.
Flammability class	Combustible IIIA estimated
Molecular formula	C ₉ H ₁₆ O ₂
Molecular weight	156.22
Oxidizing properties	Not oxidizing.
Specific gravity	0.896 - 0.902 at 25°C. Bedoukian obtained value.

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	Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	No hazardous decomposition products are known.

11. Toxicological information

Toxicological information

Notes: RIFM

Information on likely routes of exposure

Inhalation	No adverse effects due to inhalation are expected.
Skin contact	No adverse effects due to skin contact are expected.
Eye contact	Causes eye irritation.
Ingestion	Expected to be a low ingestion hazard.

Symptoms related to the physical, chemical and toxicological characteristics Irritation of eyes. Exposed individuals may experience eye tearing, redness, and discomfort.

Information on toxicological effects

Acute toxicity Not known.

Product	Species	Test Results
GUAVANATE™ (CAS 41654-15-3)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	> 5000 mg/kg Result for similar materials Methyl 9-undecenoate and Methyl 2-nonenolate.
Oral		
<i>Liquid</i>		
LD50	Rat	> 5000 mg/kg Result for similar materials Methyl 2-nonenolate and Methyl 3-nonenolate.

* 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

100 % Patch test, Result for similar material cis-3-Hexenyl
cis-3-Hexenoate.
Result: No irritation observed.
Species: Rabbit
Organ: Skin
Observation Period: 72 Hours
Notes: RIFM

**Serious eye damage/eye
irritation**

Causes eye irritation.

Irritation Corrosion - Eye

100 % Draize, 3 dose levels, 10%, 30%, 100%, vehicle
Diethyl phthalate. No cornea alterations observed at any
dose level. Weak conjunctival irritation cleared in 48 hours at
10% and 30%. Moderate conjunctival irritation clear by day 7
at 100% dose level. Result for similar material Methyl
2-nonenolate.
Result: Irritation noted.
Species: Rabbit
Organ: Eye
Observation Period: 14 days
Severity: moderate

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

Skin sensitization This product is not expected to cause skin sensitization.

Skin sensitization

Maximization test, Intradermal induction 1% in Dobbs Saline.
Topical induction 10%, vehicle ethanol; topical challenge
0.5% and 1%, vehicle ethanol. Result for similar material
Methyl 2-nonenolate.
Result: Not sensitizing.
Species: Guinea pig
Organ: Skin
Notes: RIFM
OECD 406, Intradermal induction 5% in Freund's Complete
Adjuvant/Corn oil/Saline. Topical induction and challenge
100% test material. Result for similar material cis-3-Hexenyl
cis-3-hexenoate.
Result: Not sensitizing.
Species: Guinea pig
Organ: Skin
Notes: RIFM

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

OECD 471, Strain WP2uvrA with and without metabolic
activation. Dosed up to 5000 µg/plate. Vehicle DMSO. Result
for similar material Methyl 3-hexenoate.
Result: Not mutagenic.
Species: Escherichia coli
Notes: RIFM
OECD 471, Strains TA 98, TA 100, TA 1535, and TA 1537
with and without metabolic activation. Dosed up to 5000
µg/plate. Vehicle DMSO. Result for similar material Methyl
3-hexenoate.
Result: Not mutagenic.
Species: Salmonella typhimurium
Notes: RIFM

Germ cell mutagenicity: Micronucleus

OECD 487, Human peripheral blood lymphocytes tested with
and without metabolic activation. Result for similar material
Methyl 3-hexenoate.
Result: Not clastogenic.
Species: Human
Organ: In vitro
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.

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

3.105, 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 - Yes
	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)	No
Canada	Domestic Substances List (DSL)	No
Canada	Non-Domestic Substances List (NDSL)	Yes
China	Inventory of Existing Chemical Substances in China (IECSC)	No
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	No
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	No
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	No
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
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).

16. Other information, including date of preparation or last revision**Issue date** 05-June-2022**Revision date** 11-August-2026**Version #** 02**Disclaimer** Bedoukian Research Inc (BRI) 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

Identification: Recommended restrictions
Physical & Chemical Properties: Multiple Properties
Toxicological Information: Toxicological Property Data

BEDOUKIAN®