

SAFETY DATA SHEET

1. Identification

Product identifier	GUAVANATE		
Other means of identification			
BRI Product Code	493		
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	Not for use in Tobacco or Nicotine delivery device applications and/or products.		
Manufacturer/Importer/Supplier/Distributor information			
Manufacturer			
Company name	Bedoukian Research		
Address	21 Finance 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	Chemtec (North America)	1-800-424-9300	
	Chemtec (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 flames and hot surfaces-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 local/regional/national/international 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	%
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 (CO ₂).
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. Cover with plastic sheet to prevent spreading. 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.
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	No exposure limits noted for ingredient(s).
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. Suitable gloves can be recommended by the glove supplier.
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	162 °F (72 °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	Hazardous polymerization does not occur.
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

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-nonenoate.
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-nonenoate.
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, Strains TA 1535, TA 1537, TA 98, TA 100, and TA 102 with and without metabolic activation. Dosed up to 5000 µg/plate. Vehicle DMSO. Result for similar materials Methyl 2-noenoate and cis-3-Hexenyl cis-3-Hexenoate.
Result: Not mutagenic.
Species: Salmonella typhimurium
Notes: RIFM

Carcinogenicity This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.

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****US. California Controlled Substances. CA Department of Justice (California Health and Safety Code Section 11100)**

Not listed.

US. Massachusetts RTK - Substance List

Not regulated.

US. New Jersey Worker and Community Right-to-Know Act

Not listed.

US. Pennsylvania Worker and Community Right-to-Know Law

Not listed.

US. Rhode Island RTK

Not regulated.

US. California Proposition 65

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)	No
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
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** 05-25-2015**Revision date** 03-22-2016**Version #** 05**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

Identification: Use limitations
Hazard(s) identification: Prevention
Physical & Chemical Properties: Multiple Properties
Physical and chemical properties: Oxidizing properties
Physical and chemical properties: Explosive properties
Stability and reactivity: Possibility of hazardous reactions
Toxicological Information: Toxicological Property Data
Ecological information: Persistence / degradability
Transport Information: Material Transportation Information
Regulatory information: US federal regulations
Other information, including date of preparation or last revision: Further information
HazReg Data: International Inventories
GHS: Classification