

SAFETY DATA SHEET

1. Identification

Product identifier	ETHYL 2-METHYL-3 AND -4-PENTENOATES	
Other means of identification		
BRI Product Code	511	
FEMA number	APPR	
Synonyms	Contains 64% FEMA/GRAS # 3456 and 33% FEMA/GRAS # 3489 * 3-Pentenoic acid, 2-methyl-, ethyl ester [1617-23-8] and 4-Pentenoic acid, 2-methyl-, ethyl ester [53399-81-8]	
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	Chemtrec (North America)	1-800-424-9300
	Chemtrec (International)	1-703-527-3887

2. Hazard(s) identification

Physical hazards	Flammable liquids	Category 3
Health hazards	Not classified.	
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Warning
Hazard statement	Flammable liquid and vapor.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Keep container tightly closed. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Wear protective gloves/eye protection/face protection.
Response	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. 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

Mixtures

Material name: ETHYL 2-METHYL-3 AND -4-PENTENOATES
511 Version #: 01 Issue date: 05-22-2017

Chemical name	Common name and synonyms	CAS number	%
CEREZOATE	3-Pentenoic acid, 2-methyl-, ethyl ester ETHYL 2-METHYL-3-PENTENOATE (HIGH CIS) Ethyl 2-methyl-cis-3-pentenoate Ethyl 2-methyl-z-3-pentenoate	1617-23-8	64
ETHYL 2-METHYL-4-PENTENOATE	4-Pentenoic acid, 2-methyl-, ethyl ester	53399-81-8	33
ETHYL 2-METHYL PENTANOATE	ETHYL 2-METHYL VALERATE Ethyl 2-Methylpentanoate Ethyl 2-methylvalerate Manzanate Pentanoic acid, 2-methyl-, ethyl ester	39255-32-8	3

Stabilizers	Common name and synonyms	CAS number	%
Chemical name			
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	Take off immediately all contaminated clothing. Rinse skin with water/shower. 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. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Direct contact with eyes may cause temporary irritation.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically. Thermal burns: Flush with water immediately. While flushing, remove clothes which do not adhere to affected area. Call an ambulance. Continue flushing during transport to hospital.
General information	Take off all contaminated clothing immediately. Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. Wash contaminated clothing before reuse.

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	Vapors may form explosive mixtures with air. Vapors may travel considerable distance to a source of ignition and flash back. 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	Flammable liquid and vapor.

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. Ventilate closed spaces before entering them. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.
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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. Take precautionary measures against static discharge. Use only non-sparking tools.

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. 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. Avoid discharge into drains, water courses or onto the ground.

Environmental precautions

7. Handling and storage

Precautions for safe handling

Do not handle, store or open near an open flame, sources of heat or sources of ignition. Protect material from direct sunlight. When using do not smoke. Explosion-proof general and local exhaust ventilation. Take precautionary measures against static discharges. All equipment used when handling the product must be grounded. Use non-sparking tools and explosion-proof equipment. 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. Prevent electrostatic charge build-up by using common bonding and grounding techniques. 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

Explosion-proof general and local exhaust ventilation.

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

ethereal, fruity odor.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

320 °F (160 °C) estimated

Flash point

110 °F (43 °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	1.75 mm Hg at 20°C estimated
Vapor density	> 1 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	2.57 estimated
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.
Other information	
Density	0.883 - 0.893 g/cm ³
Explosive properties	Not explosive.
Flammability class	Combustible II estimated
Oxidizing properties	Not oxidizing.
Specific gravity	0.883 - 0.893 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	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

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	Direct contact with eyes may cause temporary irritation.
Ingestion	Expected to be a low ingestion hazard.

Symptoms related to the physical, chemical and toxicological characteristics Direct contact with eyes may cause temporary irritation.

Information on toxicological effects

Acute toxicity

Components	Species	Test Results
CEREZOATE (CAS 1617-23-8)		
<u>Acute</u>		
Oral		
<i>Liquid</i>		
LD50	Rat	> 5000 mg/kg

Components	Species	Test Results
ETHYL 2-METHYL PENTANOATE (CAS 39255-32-8)		
Acute		
Oral		
<i>Liquid</i>		
LD50	Rat	> 5 ml/kg
ETHYL 2-METHYL-4-PENTENOATE (CAS 53399-81-8)		
Acute		
Oral		
<i>Liquid</i>		
LD50	Rat	> 5000 mg/kg Result for similar material Ethyl 2-methyl-3-pentenoate.

* 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

ETHYL 2-METHYL PENTANOATE

100 % OECD 404, Very slight or well-defined erythema, very slight or slight scaliness, and very slight edema in 3/3 animals. After 14 days, all skin effects had cleared completely.

Result: Irritation noted.

Species: Rabbit

Organ: Skin

Notes: ECHA

CEREZOATE

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

ETHYL 2-METHYL-4-PENTENOATE

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 Direct contact with eyes may cause temporary irritation.

Irritation Corrosion - Eye

ETHYL 2-METHYL PENTANOATE

100 % OECD 405, Slight redness and slight swelling of the conjunctivae. After 48 hours, all eye effects had cleared completely.

Result: Not irritating.

Species: Rabbit

Organ: Eye

Notes: ECHA

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

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

Skin sensitization

CEREZOATE

25 % Maximization test, Intradermal induction 25% in Freund's Complete Adjuvant/Propylene glycol. Topical induction and challenge 25% in Petrolatum. Result for similar material Ethyl 2-methylpentanoate.

Result: Not sensitizing.

Species: Guinea pig

Organ: Skin

Notes: RIFM

Skin sensitization

ETHYL 2-METHYL-4-PENTENOATE

25 % Maximization test, Intradermal induction 25% in Freund's Complete Adjuvant/Propylene glycol. Topical induction and challenge 25% in Petrolatum. Result for similar material Ethyl 2-methylpentanoate.

Result: Not sensitizing.

Species: Guinea pig

Organ: Skin

Notes: RIFM

ETHYL 2-METHYL PENTANOATE

25 % Maximization test, Intradermal induction 25% in Freund's Complete Adjuvant/Propylene glycol. Topical induction and challenge 25% in Petrolatum.

Result: Not sensitizing.

Species: Guinea pig

Organ: Skin

Notes: RIFM

CEREZOATE

5 % 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

ETHYL 2-METHYL-4-PENTENOATE

5 % 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

CEREZOATE

< 5000 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100 with and without metabolic activation. Vehicle DMSO. Result for similar material Ethyl-2-methylpentanoate.

Result: Not mutagenic.

Species: Salmonella typhimurium

Notes: RIFM

ETHYL 2-METHYL-4-PENTENOATE

< 5000 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100 with and without metabolic activation. Vehicle DMSO. Result for similar material Ethyl-2-methylpentanoate.

Result: Not mutagenic.

Species: Salmonella typhimurium

Notes: RIFM

ETHYL 2-METHYL PENTANOATE

< 5000 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100 with and without metabolic activation. Vehicle DMSO.

Result: Not mutagenic.

Species: Salmonella typhimurium

Notes: RIFM

CEREZOATE

33 - 5000 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100, and TA 102 with and without metabolic activation. Vehicle DMSO. Result for similar material cis-3-Hexenyl cis-3-Hexenoate.

Result: Not mutagenic.

Species: Salmonella typhimurium

Notes: RIFM

ETHYL 2-METHYL-4-PENTENOATE

33 - 5000 µg/plate, Strains TA 1535, TA 1537, TA 98, TA 100, and TA 102 with and without metabolic activation. Vehicle DMSO. Result for similar material 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)

ETHYL 2-METHYL-3 AND -4-PENTENOATES
CEREZOATE

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

ETHYL 2-METHYL PENTANOATE

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

ETHYL 2-METHYL-4-PENTENOATE

2.62, 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	
UN number	UN1993
UN proper shipping name	Flammable liquid, n.o.s. (ETHYL 2-METHYL-3&4-PENTENOATES)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	III
Environmental hazards	No.
ERG Code	3L
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.

Other information

Passenger and cargo aircraft Allowed with restrictions.
Cargo aircraft only Allowed with restrictions.

IMDG

UN number UN1993
UN proper shipping name FLAMMABLE LIQUID, N.O.S. (ETHYL 2-METHYL-3&4-PENTENOATES)
Transport hazard class(es)
Class 3
Subsidiary risk -
Packing group III
Environmental hazards
Marine pollutant No.
EmS F-E, S-E
Special precautions for user Read safety instructions, SDS and emergency procedures before handling.

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

IATA; IMDG



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 - No
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)	Yes
Canada	Domestic Substances List (DSL)	No
Canada	Non-Domestic Substances List (NDSL)	Yes
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)	No
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	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** 05-22-2017**Version #** 01**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

Physical & Chemical Properties: Multiple Properties
 Physical and chemical properties: Oxidizing properties
 Physical and chemical properties: Explosive properties
 Ecological information: Persistence / degradability
 Other information, including date of preparation or last revision: Further information