

1. Identification

Product identifier ETHYL 2-METHYL-4-PENTENOATE

Other means of identification

BRI Product Code 436

CAS number 53399-81-8

FEMA number 3489

Synonyms 4-Pentenoic acid, 2-methyl-, ethyl ester

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 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 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	%
ETHYL 2-METHYL-4-PENTENOATE	4-Pentenoic acid, 2-methyl-, ethyl ester	53399-81-8	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	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.
Methods and materials for containment and cleaning up	Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). Take precautionary measures against static discharge. Use only non-sparking tools. 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. 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

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

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

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

pineapple odor; similar to a tiglato.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

311.83 °F (155.46 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Flash point

108 °F (42 °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

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

Vapor density

4.9 Relative to air; air = 1

Relative density

Not available.

Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	2.62 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	0.880 - 0.886 g/cm3
Flammability class	Combustible II estimated
Molecular formula	C8H14O2
Molecular weight	142.19
Specific gravity	0.88 - 0.886 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	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

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

Product	Species	Test Results
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-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.

Respiratory or skin sensitization

Respiratory sensitization Not a respiratory sensitizer.

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

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

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

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

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-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-4-PENTENOATE)
Transport hazard class(es)
 Class 3
 Subsidiary risk -
 Label(s) 3
Packing group III
Environmental hazards No.
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-4-PENTENOATE)
Transport hazard class(es)
 Class 3
 Subsidiary risk -
 Label(s) 3
Packing group III
Environmental hazards
 Marine pollutant No.
EmS Not available.
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.

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
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 21-May-2015

Revision date 12-June-2020

Version # 04

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

Hazard(s) identification: Disposal

Physical & Chemical Properties: Multiple Properties

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