

1. Identification

Product identifier cis-3-HEXENYL TIGLATE

Other means of identification

BRI Product Code 116

CAS number 67883-79-8

FEMA number 3931

Synonyms (Z)-3-hexenyl 2-methylcrotonate * 2-Butenoic acid, 2-methyl-, (3Z)-3-hexenyl ester, (2E)- * C-3-HEXENYL TIGLATE * Z-3-Hexenyl tiglate

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

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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 Not classified.

Environmental hazards Not classified.

OSHA defined hazards Not classified.

Label elements

Hazard symbol None.

Signal word None.

Hazard statement The substance does not meet the criteria for classification.

Precautionary statement

Prevention Observe good industrial hygiene practices.

Response Wash hands after handling.

Storage Store away from incompatible materials.

Disposal Dispose of waste and residues in accordance with local authority requirements.

Hazard(s) not otherwise classified (HNOC) None known.

Supplemental information 100% of the mixture consists of component(s) of unknown acute inhalation toxicity. 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	%
cis-3-HEXENYL TIGLATE	(Z)-3-hexenyl 2-methylcrotonate 2-Butenoic acid, 2-methyl-, (3Z)-3-hexenyl ester, (2E)-C-3-HEXENYL TIGLATE Z-3-Hexenyl tiglate	67883-79-8	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	Wash off with soap and water. Get medical attention if irritation develops and persists.
Eye contact	Rinse with water. 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	Treat symptomatically.
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	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. 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	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	Wear safety glasses with side shields (or goggles).
Skin protection	
Hand protection	Wear appropriate chemical resistant gloves. Select suitable chemical resistant protective gloves (EN 374) with a protective index 6 (>480min permeation time).
Other	Wear suitable protective clothing.
Respiratory protection	In case of insufficient ventilation, wear suitable respiratory equipment.
Thermal hazards	Wear appropriate thermal protective clothing, when necessary.
General hygiene considerations	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	fresh, green, floral, fruity odor.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	456.75 °F (235.97 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Flash point	210 °F (99 °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	0.04 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	6.3 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	3.93 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	0.910 - 0.918 g/cm3
Explosive properties	Not explosive.

Flammability class	Combustible IIIB estimated
Molecular formula	C11H18O2
Molecular weight	182.27
Oxidizing properties	Not oxidizing.
Specific gravity	0.91 - 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	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 Not known.

Product	Species	Test Results
cis-3-HEXENYL TIGLATE (CAS 67883-79-8)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	> 5000 mg/kg
Oral		
<i>Liquid</i>		
LD50	Rat	> 5000 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

cis-3-HEXENYL TIGLATE

12 % Patch test, Vehicle Petrolatum.

Result: No irritation observed.

Species: Human

Organ: Skin

Notes: RIFM

5000 mg/kg LD50, Irritation evaluated on day 1 of an LD50 study, 10 animals evaluated. Moderate erythema in 10; moderate edema in 10.

Result: Irritation noted.

Species: Rabbit

Organ: Skin

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

cis-3-HEXENYL TIGLATE

12 % Patch test, Vehicle Petrolatum.

Result: Not sensitizing.

Species: Human

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

cis-3-HEXENYL TIGLATE

< 5000 µg/plate Plate incorporation, Strains TA 1535, TA 1537, TA 98, and TA 100 with and without metabolic activation. Result for similar material Hexyl tiglate.

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 The product is readily biodegradable.

Biodegradability

Percent degradation (Aerobic biodegradation-ready)

cis-3-HEXENYL TIGLATE

30 mg/l OECD 301F

Result: Readily biodegradable.

Species: Activated sludge of a predominantly domestic sewage

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

cis-3-HEXENYL TIGLATE

3.93, 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.

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 not known to be 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 - No
Pressure Hazard - No
Reactivity Hazard - No

SARA 302 Extremely hazardous substance

Not listed.

SARA 311/312 Hazardous chemical No

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)	No
New Zealand	New Zealand Inventory	Yes

Country(s) or region	Inventory name	On inventory (yes/no)*
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	05-October-2018
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	Accidental release measures: Personal precautions, protective equipment and emergency procedures Accidental release measures: Methods and materials for containment and cleaning up Handling and storage: Conditions for safe storage, including any incompatibilities Ecological Information: Ecotox Property Data Ecological information: Persistence / degradability