

**1. Identification**

<b>Product identifier</b>	<b>cis-3-HEXENYL CAPROATE (HEXANOATE)</b>		
<b>Other means of identification</b>			
<b>BRI Product Code</b>	108		
<b>CAS number</b>	31501-11-8		
<b>FEMA number</b>	3403		
<b>Synonyms</b>	(Z)-Hex-3-enyl hexanoate * C-3-Hexenyl caproate * Hexanoic acid, (3Z)-3-hexenyl ester * Z-3-Hexenyl caproate		
<b>Recommended use</b>	flavors and fragrances For Manufacturing Use Only		
<b>Recommended restrictions</b>	Not for use in Tobacco or Nicotine delivery device applications and/or products.		
<b>Manufacturer/Importer/Supplier/Distributor information</b>			
<b>Manufacturer</b>			
<b>Company name</b>	Bedoukian Research		
<b>Address</b>	6 Commerce Drive Danbury, CT 06810 United States		
<b>Telephone</b>	1-203-830-4000		
<b>Website</b>	www.bedoukian.com		
<b>E-mail</b>	customerservice@bedoukian.com		
<b>Contact person</b>	Joseph Bania		
<b>Emergency phone number</b>	Chemtrec (North America)	1-800-424-9300	
	Chemtrec (International)	1-703-527-3887	

**2. Hazard(s) identification**

<b>Physical hazards</b>	Not classified.
<b>Health hazards</b>	Not classified.
<b>Environmental hazards</b>	Not classified.
<b>OSHA defined hazards</b>	Not classified.
<b>Label elements</b>	
<b>Hazard symbol</b>	None.
<b>Signal word</b>	None.
<b>Hazard statement</b>	The substance does not meet the criteria for classification.
<b>Precautionary statement</b>	
<b>Prevention</b>	Observe good industrial hygiene practices.
<b>Response</b>	Wash hands after handling.
<b>Storage</b>	Store away from incompatible materials.
<b>Disposal</b>	Dispose of waste and residues in accordance with local authority requirements.
<b>Hazard(s) not otherwise classified (HNOC)</b>	None known.
<b>Supplemental information</b>	None.

**3. Composition/information on ingredients**

**Substances**

Chemical name	Common name and synonyms	CAS number	%
cis-3-HEXENYL CAPROATE (HEXANOATE)	(Z)-Hex-3-enyl hexanoate C-3-Hexenyl caproate Hexanoic acid, (3Z)-3-hexenyl ester Z-3-Hexenyl caproate	31501-11-8	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

<b>Inhalation</b>	Move to fresh air. Call a physician if symptoms develop or persist.
<b>Skin contact</b>	Wash off with soap and water. Get medical attention if irritation develops and persists.
<b>Eye contact</b>	Rinse with water. Get medical attention if irritation develops and persists.
<b>Ingestion</b>	Rinse mouth. Get medical attention if symptoms occur.
<b>Most important symptoms/effects, acute and delayed</b>	Direct contact with eyes may cause temporary irritation.
<b>Indication of immediate medical attention and special treatment needed</b>	Treat symptomatically.
<b>General information</b>	Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves.

### 5. Fire-fighting measures

<b>Suitable extinguishing media</b>	Water fog. Foam. Dry chemical powder. Carbon dioxide (CO <sub>2</sub> ).
<b>Unsuitable extinguishing media</b>	Do not use water jet as an extinguisher, as this will spread the fire.
<b>Specific hazards arising from the chemical</b>	During fire, gases hazardous to health may be formed.
<b>Special protective equipment and precautions for firefighters</b>	Self-contained breathing apparatus and full protective clothing must be worn in case of fire.
<b>Fire fighting equipment/instructions</b>	Move containers from fire area if you can do so without risk.
<b>Specific methods</b>	Use standard firefighting procedures and consider the hazards of other involved materials.
<b>General fire hazards</b>	No unusual fire or explosion hazards noted.

### 6. Accidental release measures

<b>Personal precautions, protective equipment and emergency procedures</b>	Keep unnecessary personnel away. For personal protection, see section 8 of the SDS.
<b>Methods and materials for containment and cleaning up</b>	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. 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.  Never return spills to original containers for re-use. For waste disposal, see section 13 of the SDS.
<b>Environmental precautions</b>	Avoid discharge into drains, water courses or onto the ground.

### 7. Handling and storage

<b>Precautions for safe handling</b>	Observe good industrial hygiene practices.
<b>Conditions for safe storage, including any incompatibilities</b>	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

<b>Occupational exposure limits</b>	This substance has no PEL, TLV, or other recommended exposure limit.
<b>Biological limit values</b>	No biological exposure limits noted for the ingredient(s).
<b>Appropriate engineering controls</b>	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

<b>Eye/face protection</b>	Wear safety glasses with side shields (or goggles).
<b>Skin protection</b>	
<b>Hand protection</b>	Wear appropriate chemical resistant gloves. Suitable gloves can be recommended by the glove supplier.
<b>Other</b>	Wear suitable protective clothing.
<b>Respiratory protection</b>	In case of insufficient ventilation, wear suitable respiratory equipment.
<b>Thermal hazards</b>	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

<b>Physical state</b>	Liquid.
<b>Color</b>	Colorless

**Odor** fruity, green pear-like odor.

**Odor threshold** Not available.

**pH** Not available.

**Melting point/freezing point** Not available.

**Initial boiling point and boiling range** 487.6 °F (253.11 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

**Flash point** 220 °F (104 °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** 0.01 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

**Vapor density** 6.8 Relative to air; air = 1

**Relative density** Not available.

### Solubility(ies)

**Solubility (water)** Not available.

**Partition coefficient (n-octanol/water)** 4.58 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** 0.873 - 0.883 g/cm<sup>3</sup>

**Flammability class** Combustible IIIB estimated

**Molecular formula** C<sub>12</sub>H<sub>22</sub>O<sub>2</sub>

**Molecular weight** 198.31

**Specific gravity** 0.873 - 0.883 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.

<b>Possibility of hazardous reactions</b>	No dangerous reaction known under conditions of normal use.
<b>Conditions to avoid</b>	Contact with incompatible materials.
<b>Incompatible materials</b>	Strong oxidizing agents.
<b>Hazardous decomposition products</b>	No hazardous decomposition products are known.

## 11. Toxicological information

### Information on likely routes of exposure

<b>Inhalation</b>	No adverse effects due to inhalation are expected.
<b>Skin contact</b>	No adverse effects due to skin contact are expected.
<b>Eye contact</b>	Direct contact with eyes may cause temporary irritation.
<b>Ingestion</b>	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
cis-3-HEXENYL CAPROATE (HEXANOATE) (CAS 31501-11-8)		
<b>Acute</b>		
<b>Dermal</b>		
<i>Liquid</i>		
LD50	Rabbit	> 5000 mg/kg
<b>Oral</b>		
<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 CAPROATE (HEXANOATE)	2 % 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. Slight erythema in 7, moderate erythema in 3; slight edema in 9. Result: Irritation noted. Species: Rabbit Organ: Skin Notes: RIFM
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**Serious eye damage/eye irritation** Direct contact with eyes may cause temporary irritation.

#### Respiratory or skin sensitization

<b>Respiratory sensitization</b>	Not a respiratory sensitizer.
<b>Skin sensitization</b>	This product is not expected to cause skin sensitization.

#### Skin sensitization

cis-3-HEXENYL CAPROATE (HEXANOATE)	2 % Patch test, Vehicle Petrolatum. Result: Not sensitizing. Species: Human Organ: Skin Notes: RIFM
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**Germ cell mutagenicity** No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.

**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)

cis-3-HEXENYL CAPROATE (HEXANOATE)

4.58, 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.

**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)	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** 19-May-2015  
**Revision date** 28-September-2018  
**Version #** 03

**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: Recommended restrictions