

1. Identification

Product identifier	cis-3-HEXENYL ISOBUTYRATE	
Other means of identification		
BRI Product Code	107	
CAS number	41519-23-7	
FEMA number	3929	
Synonyms	(Z)-hex-3-enyl isobutyrate * C-3-HEXENYL ISOBUTYRATE * Propanoic acid, 2-methyl-, (3Z)-3-hexenyl ester * Verdural B Extra * Z-3-Hexenyl isobutyrate	
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 4
Health hazards	Not classified.	
Environmental hazards	Hazardous to the aquatic environment, acute hazard	Category 2
OSHA defined hazards	Not classified.	
Label elements		
Hazard symbol	None.	
Signal word	Warning	
Hazard statement	Combustible liquid. Toxic to aquatic life.	
Precautionary statement		
Prevention	Keep away from flames and hot surfaces-No smoking. Avoid release to the environment. Wear protective gloves/eye protection/face protection.	
Response	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	%
cis-3-HEXENYL ISOBUTYRATE	(Z)-hex-3-enyl isobutyrate C-3-HEXENYL ISOBUTYRATE Propanoic acid, 2-methyl-, (3Z)-3-hexenyl ester Verdural B Extra Z-3-Hexenyl isobutyrate	41519-23-7	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	Provide general supportive measures and 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	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. 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. Prevent product from entering drains. Large Spills: Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible. 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 release to the environment. Inform appropriate managerial or supervisory personnel of all environmental releases. Prevent further leakage or spillage if safe to do so. 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. Provide adequate ventilation. Wear appropriate personal protective equipment. Avoid release to the environment. 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

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

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

green, fruity, apple-like odor.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

Not available.

Initial boiling point and boiling range

400.89 °F (204.94 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

Flash point

160 °F (71 °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

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

Vapor density

5.9 Relative to air; air = 1

Relative density

Not available.

Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	3.52 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	0.874 - 0.884 g/cm3
Explosive properties	Not explosive.
Flammability class	Combustible IIIA estimated
Molecular formula	C10H18O2
Molecular weight	170.25
Oxidizing properties	Not oxidizing.
Specific gravity	0.874 - 0.884 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

Product	Species	Test Results
cis-3-HEXENYL ISOBUTYRATE (CAS 41519-23-7)		
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 ISOBUTYRATE

10 % Patch test, Vehicle Petrolatum.
Result: No irritation observed.
Species: Human
Organ: Skin
Notes: RIFM
100 OECD 439
Result: Not irritating.
Organ: In vitro
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 ISOBUTYRATE

10 % 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 ISOBUTYRATE

< 1250 µg/plate, Strain WP2uvrA with and without metabolic activation. Vehicle DMSO. Result for similar material cis-3-Hexenyl methyl carbonate.
Result: Not mutagenic.
Species: Escherichia coli
Notes: RIFM
< 1250 µg/plate, Strains TA 1535, TA 1537, TA 98, and TA 100 with and without metabolic activation. Vehicle DMSO.
Result for similar material cis-3-Hexenyl methyl carbonate.
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 Toxic to aquatic life.

Product	Species		Test Results
cis-3-HEXENYL ISOBUTYRATE (CAS 41519-23-7)			
Aquatic			
<i>Acute</i>			
Algae	EC50	Algae	5.3 mg/l, 72 h OECD 201
Crustacea	EC50	Daphnia	20 mg/l, 48 h OECD 202

* Estimates for product may be based on additional component data not shown.

Persistence and degradability No data is available on the degradability of this product.

Biodegradability

Percent degradation (Aerobic biodegradation-ready)

cis-3-HEXENYL ISOBUTYRATE

OECD 301F, 30 mg/L. 10-day criteria fulfilled.
Result: Readily biodegradable.
Species: Activated sludge of a predominantly domestic sewage

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

cis-3-HEXENYL ISOBUTYRATE

3.52, 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. Do not allow this material to drain into sewers/water supplies. Do not contaminate ponds, waterways or ditches with chemical or used container. 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 - 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

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
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 16-May-2015
Revision date 03-January-2020
Version # 06

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: Hazard statement
Hazard(s) identification: Disposal
Hazard(s) identification: Prevention
Composition/information on ingredients: Composition comments
Accidental release measures: Personal precautions, protective equipment and emergency procedures
Accidental release measures: Environmental precautions
Accidental release measures: Methods and materials for containment and cleaning up
Stability and reactivity: Possibility of hazardous reactions
Toxicological Information: Toxicological Property Data
Ecological Information: Ecotoxicity
Ecological information: Ecotoxicity
Ecological information: Persistence / degradability
Disposal considerations: Disposal instructions
Material Attributes & Uses; Experimental Data: Experimental Data

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