

**1. Identification**

<b>Product identifier</b>	<b>2,4-HEXADIENYL ISOBUTYRATE</b>	
<b>Other means of identification</b>		
<b>BRI Product Code</b>	223	
<b>FEMA number</b>	4134	
<b>Synonyms</b>	Hexa-2,4-dienyl isobutyrate * Propanoic acid, 2-methyl-, 2,4-hexadienyl ester * Sorbyl isobutyrate	
<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>	21 Finance 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>	Flammable liquids	Category 4
<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>	Warning	
<b>Hazard statement</b>	Combustible liquid.	
<b>Precautionary statement</b>		
<b>Prevention</b>	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Wear protective gloves/eye protection/face protection.	
<b>Response</b>	In case of fire: Use appropriate media to extinguish.	
<b>Storage</b>	Store in a well-ventilated place. Keep cool.	
<b>Disposal</b>	Dispose of contents/container in accordance with local/regional/national/international regulations.	
<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	%
2,4-HEXADIENYL ISOBUTYRATE	Hexa-2,4-dienyl isobutyrate Propanoic acid, 2-methyl-, 2,4-hexadienyl ester Sorbyl isobutyrate	16491-24-0	100

## Stabilizers

Chemical name	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>	Provide general supportive measures and 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>	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.
<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>	In case of fire and/or explosion do not breathe fumes. 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>	Combustible liquid.

## 6. Accidental release measures

<b>Personal precautions, protective equipment and emergency procedures</b>	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.
<b>Methods and materials for containment and cleaning up</b>	Eliminate all ignition sources (no smoking, flares, sparks, or flames in immediate area). 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.
<b>Environmental precautions</b>	Avoid discharge into drains, water courses or onto the ground.

## 7. Handling and storage

<b>Precautions for safe handling</b>	Keep away from open flames, hot surfaces and sources of ignition. When using do not smoke. Provide adequate ventilation. Wear appropriate personal protective equipment. Observe good industrial hygiene practices.
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**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** No exposure limits noted for ingredient(s).

**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. 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 to pale yellow

**Odor** green apple, somewhat herbaceous.

**Odor threshold** Not available.

**pH** Not available.

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

**Initial boiling point and boiling range** 411.73 °F (210.96 °C) US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

**Flash point** 180 °F (82 °C) Pensky-Martens or Grabner Miniflash

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

**Vapor density** 5.8 Relative to air; air = 1

**Relative density** Not available.

**Solubility(ies)**

**Solubility (water)** Not available.

**Partition coefficient (n-octanol/water)** 3.31 US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.

<b>Auto-ignition temperature</b>	Not available.
<b>Decomposition temperature</b>	Not available.
<b>Viscosity</b>	Not available.
<b>Other information</b>	
<b>Density</b>	0.902 - 0.906 g/cm <sup>3</sup>
<b>Flammability class</b>	Combustible IIIA estimated
<b>Molecular formula</b>	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
<b>Molecular weight</b>	168.24
<b>Specific gravity</b>	0.902 - 0.906 at 25°C

## 10. Stability and reactivity

<b>Reactivity</b>	The product is stable and non-reactive under normal conditions of use, storage and transport.
<b>Chemical stability</b>	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>	Avoid heat, sparks, open flames and other ignition sources. Avoid temperatures exceeding the flash point. 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
2,4-HEXADIENYL ISOBUTYRATE (CAS 16491-24-0)		
<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.

<b>Skin corrosion/irritation</b>	Prolonged skin contact may cause temporary irritation.
<b>Serious eye damage/eye irritation</b>	Direct contact with eyes may cause temporary irritation.
<b>Respiratory or skin sensitization</b>	
<b>Respiratory sensitization</b>	Not a respiratory sensitizer.
<b>Skin sensitization</b>	This product is not expected to cause skin sensitization.
<b>Germ cell mutagenicity</b>	No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.
<b>Carcinogenicity</b>	This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.

## OSHA Specifically Regulated Substances (29 CFR 1910.1001-1050)

Not listed.

<b>Reproductive toxicity</b>	This product is not expected to cause reproductive or developmental effects.
<b>Specific target organ toxicity - single exposure</b>	Not classified.
<b>Specific target organ toxicity - repeated exposure</b>	Not classified.
<b>Aspiration hazard</b>	Not an aspiration hazard.

## 12. Ecological information

<b>Ecotoxicity</b>	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.
<b>Persistence and degradability</b>	No data is available on the degradability of this product.

### Bioaccumulative potential

#### Partition coefficient n-octanol / water (log Kow)

2,4-HEXADIENYL ISOBUTYRATE

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

<b>Mobility in soil</b>	No data available.
<b>Other adverse effects</b>	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

<b>Disposal instructions</b>	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.
<b>Local disposal regulations</b>	Dispose in accordance with all applicable regulations.
<b>Hazardous waste code</b>	The waste code should be assigned in discussion between the user, the producer and the waste disposal company.
<b>Waste from residues / unused products</b>	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).
<b>Contaminated packaging</b>	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 listed.

## 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)	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)	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** 05-29-2015  
**Version #** 01

**Disclaimer**

BRI 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.

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