

SAFETY DATA SHEET

1. Identification

Product identifier	cis-3-HEXENAL (50% IN TRIACETIN)	
Other means of identification		
BRI Product Code	375	
FEMA number	APPR	
Synonyms	Contains 50% FEMA/GRAS # 2561 * 3-Hexenal, (3Z)- [6789-80-6] in 1,2,3-Propanetriol, triacetate [102-76-1] * cis-3-Hexen-1-ol	
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	Acute toxicity, oral	Category 4
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	

Label elements



Signal word	Warning
Hazard statement	Flammable liquid and vapor. Harmful if swallowed.
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. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Wear protective gloves/eye protection/face protection.
Response	If swallowed: Call a poison center/doctor if you feel unwell. Rinse mouth. 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)	Static accumulating flammable liquid can become electrostatically charged even in bonded and grounded equipment. Sparks may ignite liquid and vapor. May cause flash fire or explosion.

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**Mixtures**

Chemical name	Common name and synonyms	CAS number	%
cis-3-HEXENAL (NEAT)	3-Hexenal, (3Z)-cis-3-Hexen-1-al	6789-80-6	50
TRIACETIN	1,2,3-Propanetriol, triacetate Glycerin triacetate Glyceryl triacetate	102-76-1	50

Stabilizers

Chemical name	Common name and synonyms	CAS number	%
synthetic alpha tocopherol		10191-41-0	0.25

*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. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Get medical advice/attention if you feel unwell.

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. Keep victim warm. Keep victim under observation. Symptoms may be delayed.

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. Show this safety data sheet to the doctor in attendance. Wash contaminated clothing before reuse.

5. Fire-fighting measures**Suitable extinguishing media**

Water fog. Foam. Carbon dioxide (CO₂). Dry chemical powder, carbon dioxide, sand or earth may be used for small fires only.

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. This product is a poor conductor of electricity and can become electrostatically charged. If sufficient charge is accumulated, ignition of flammable mixtures can occur. To reduce potential for static discharge, use proper bonding and grounding procedures. This liquid may accumulate static electricity when filling properly grounded containers. Static electricity accumulation may be significantly increased by the presence of small quantities of water or other contaminants. Material will float and may ignite on surface of water. 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. Use appropriate containment to avoid environmental contamination. Transfer by mechanical means such as vacuum truck to a salvage tank or other suitable container for recovery or safe disposal. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS. 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. Take precautionary measures against static discharge. Use only non-sparking tools.

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. 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. For waste disposal, see section 13 of the SDS.

Environmental precautions

Avoid discharge into drains, water courses or onto the ground. Use appropriate containment to avoid environmental contamination.

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. Explosion-proof general and local exhaust ventilation. Minimize fire risks from flammable and combustible materials (including combustible dust and static accumulating liquids) or dangerous reactions with incompatible materials. Handling operations that can promote accumulation of static charges include but are not limited to: mixing, filtering, pumping at high flow rates, splash filling, creating mists or sprays, tank and container filling, tank cleaning, sampling, gauging, switch loading, vacuum truck operations. Take precautionary measures against static discharges. All equipment used when handling the product must be grounded. Use non-sparking tools and explosion-proof equipment. Do not taste or swallow. When using, do not eat, drink or smoke. Wear appropriate personal protective equipment. Wash hands thoroughly after handling. Observe good industrial hygiene practices.

For additional information on equipment bonding and grounding, refer to the Canadian Electrical Code in Canada, (CSA C22.1), or the American Petroleum Institute (API) Recommended Practice 2003, "Protection Against Ignitions Arising out of Static, Lightning, and Stray Currents" or National Fire Protection Association (NFPA) 77, "Recommended Practice on Static Electricity" or National Fire Protection Association (NFPA) 70, "National Electrical Code".

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. Eliminate sources of ignition. Avoid spark promoters. Ground/bond container and equipment. These alone may be insufficient to remove static electricity. 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). Store away from incompatible materials (see Section 10 of the SDS). Store tightly sealed under inert gas below 0 deg. C Recommended Packaging: Glass or Aluminum.

8. Exposure controls/personal protection

Occupational exposure limits

This mixture has no ingredients that have 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

Face shield is recommended. Wear safety glasses with side shields (or goggles).

Skin protection

Hand protection

Wear appropriate chemical resistant gloves.

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. Keep away from food and drink. 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	powerful, green, grassy apple-like odor.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	37.4 °F (3 °C) estimated
Initial boiling point and boiling range	Not available.
Flash point	96 °F (36 °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	5.6 hPa estimated
Vapor density	Not available.
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	Not available.
Auto-ignition temperature	812 °F (433.33 °C) estimated
Decomposition temperature	Not available.
Viscosity	Not available.

Other information

Density	0.981 g/cm ³ estimated
Explosive properties	Not explosive.
Flammability class	Flammable IC estimated
Oxidizing properties	Not oxidizing.

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	Harmful if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics Direct contact with eyes may cause temporary irritation.

Information on toxicological effects

Acute toxicity Harmful if swallowed.

Product	Species	Test Results
cis-3-HEXENAL (50% IN TRIACETIN)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	3700 mg/kg Material tested: cis-3-Hexenal 50% in Triacetin.
Oral		
<i>Liquid</i>		
LD50	Rat	1560 mg/kg Material tested: cis-3-Hexenal 50% in Triacetin.

Components	Species	Test Results
cis-3-HEXENAL (NEAT) (CAS 6789-80-6)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	3700 mg/kg Result for cis-3-Hexenal 50% in Triacetin.
Oral		
<i>Liquid</i>		
LD50	Rat	1560 mg/kg Result for cis-3-Hexenal 50% in Triacetin.
TRIACETIN (CAS 102-76-1)		
Acute		
Oral		
<i>Liquid</i>		
LD50	Rat	> 3000 mg/kg
LD50	Rat	3000 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-HEXENAL (NEAT)

2 % Patch test, Vehicle Petrolatum.
Result: No irritation observed.
Species: Human
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-HEXENAL (NEAT)

2 % 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.

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 No data is available on the degradability of this product.

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

cis-3-HEXENAL (NEAT)

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

TRIACETIN

0.25

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

UN number UN1993

UN proper shipping name Flammable liquids, n.o.s. (cis-3-HEXENAL)

Transport hazard class(es)

Class 3

Subsidiary risk -

Label(s) 3

Packing group III

Special precautions for user Read safety instructions, SDS and emergency procedures before handling. Read safety instructions, SDS and emergency procedures before handling.

Special provisions	B1, B52, IB3, T4, TP1, TP29
Packaging exceptions	150
Packaging non bulk	203
Packaging bulk	242

IATA

UN number	UN1993
UN proper shipping name	Flammable liquid, n.o.s. (cis-3-HEXENAL)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	III
Environmental hazards	No.
ERG Code	3L
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling. 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. (cis-3-HEXENAL)
Transport hazard class(es)	
Class	3
Subsidiary risk	-
Packing group	III
Environmental hazards	
Marine pollutant	No.
EmS	F-E, S-E
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling. 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.

DOT



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 - Yes
 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)	No
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 03-May-2017
Revision date 11-November-2021
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

Hazard(s) identification: Disposal
Physical & Chemical Properties: Multiple Properties

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