

SAFETY DATA SHEET

1. Identification

Product identifier	ALLYL CAPROATE (HEXANOATE) FCC	
Other means of identification		
BRI Product Code	560	
FEMA number	2032	
Synonyms	2-Propenyl hexanoate * Allyl capronate * Hexanoic acid, 2-propenyl ester * Hexanoic acid, allyl ester	
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	21 Finance 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	Acute toxicity, oral	Category 3
	Acute toxicity, dermal	Category 3
	Acute toxicity, inhalation	Category 3
	Skin corrosion/irritation	Category 2
Environmental hazards	Hazardous to the aquatic environment, acute hazard	Category 1
	Hazardous to the aquatic environment, long-term hazard	Category 3
OSHA defined hazards	Not classified.	

Label elements



Signal word	Danger
Hazard statement	Combustible liquid. Toxic if swallowed. Toxic in contact with skin. Causes skin irritation. Toxic if inhaled. Very toxic to aquatic life. Harmful to aquatic life with long lasting effects.
Precautionary statement	
Prevention	Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Avoid breathing vapors. Wash thoroughly after handling. Do not eat, drink or smoke when using this product. Use only outdoors or in a well-ventilated area. Avoid release to the environment. Wear protective gloves/protective clothing. Wear protective gloves/eye protection/face protection.

Response	If swallowed: Immediately call a poison center/doctor. If on skin: Wash with plenty of water. If inhaled: Remove person to fresh air and keep comfortable for breathing. Call a poison center/doctor. Rinse mouth. If skin irritation occurs: Get medical advice/attention. Take off immediately all contaminated clothing and wash it before reuse. In case of fire: Use appropriate media to extinguish. Collect spillage.
Storage	Store in a well-ventilated place. Keep container tightly closed. Store in a well-ventilated place. Keep cool. Store locked up.
Disposal	Dispose of contents/container in accordance with local/regional/national/international 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	%
ALLYL CAPROATE (HEXANOATE) FCC	2-Propenyl hexanoate Allyl capronate Hexanoic acid, 2-propenyl ester Hexanoic acid, allyl ester	123-68-2	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

Inhalation

Remove victim to fresh air and keep at rest in a position comfortable for breathing. Oxygen or artificial respiration if needed. Do not use mouth-to-mouth method if victim inhaled the substance. Induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Call a POISON CENTER or doctor/physician.

Skin contact

Take off immediately all contaminated clothing. Wash with plenty of soap and water. Get medical advice/attention if you feel unwell. If skin irritation occurs: Get medical advice/attention. Wash contaminated clothing before reuse.

Eye contact

Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.

Ingestion

Call a physician or poison control center immediately. Rinse mouth. Do not induce vomiting without advice from poison control center. If vomiting occurs, keep head low so that stomach content doesn't get into the lungs. Do not use mouth-to-mouth method if victim ingested the substance. Induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device.

Most important symptoms/effects, acute and delayed

Direct contact with eyes may cause temporary irritation. Skin irritation. May cause redness and pain.

Indication of immediate medical attention and special treatment needed

Provide general supportive measures and treat symptomatically. Keep victim warm. Keep victim under observation. Symptoms may be delayed.

General information

Take off immediately all contaminated clothing. 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.

5. Fire-fighting measures

Suitable extinguishing media

Water fog. Foam. Dry chemical powder. Carbon dioxide (CO₂).

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. Avoid inhalation of vapors and spray mists. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. 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.

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. Prevent product from entering drains. 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.

Environmental precautions	Avoid release to the environment. Prevent further leakage or spillage if safe to do so. Avoid discharge into drains, water courses or onto the ground. Inform appropriate managerial or supervisory personnel of all environmental releases.
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7. Handling and storage

Precautions for safe handling	Keep away from open flames, hot surfaces and sources of ignition. Avoid inhalation of vapors and spray mists. Avoid contact with eyes, skin, and clothing. Do not taste or swallow. When using, do not eat, drink or smoke. Use only outdoors or in a well-ventilated area. Wear appropriate personal protective equipment. Wash hands thoroughly after handling. Avoid release to the environment. Wash contaminated clothing before reuse. Observe good industrial hygiene practices.
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Conditions for safe storage, including any incompatibilities	Store locked up. 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.
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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. Eye wash facilities and emergency shower must be available when handling this product.

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 appropriate chemical resistant clothing. Use of an impervious apron is recommended.
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. Dust & vapor respirator.
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.
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9. Physical and chemical properties

Appearance

Physical state	Liquid.
Color	colorless to light yellow
Odor	fruity, fatty, pineapple, rum.
Odor threshold	Not available.
pH	Not available.
Melting point/freezing point	Not available.
Initial boiling point and boiling range	366.8 °F (186 °C) Literature reference.
Flash point	151 °F (66 °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	0.497 mmHg at 20°C; US EPA. 2014. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US EPA, Washington, DC, USA.
Vapor density	5.4 Relative to air; air = 1
Relative density	Not available.
Solubility(ies)	
Solubility (water)	Not available.
Partition coefficient (n-octanol/water)	3.18 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	0.884 - 0.89 g/cm ³
Flammability class	Combustible IIIA estimated
Molecular formula	C ₉ H ₁₆ O ₂
Molecular weight	156.23
Specific gravity	0.884 - 0.89 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	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	Toxic if inhaled.
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Skin contact Toxic in contact with skin. Causes skin irritation.
Eye contact Direct contact with eyes may cause temporary irritation.
Ingestion Toxic if swallowed.

Symptoms related to the physical, chemical and toxicological characteristics Skin irritation. May cause redness and pain.

Information on toxicological effects

Acute toxicity Toxic if inhaled. Toxic in contact with skin. Toxic if swallowed.

Product	Species	Test Results
ALLYL CAPROATE (HEXANOATE) FCC (CAS 123-68-2)		
Acute		
Dermal		
<i>Liquid</i>		
LD50	Rabbit	820 mg/kg
Oral		
<i>Liquid</i>		
LD50	Rat	218 mg/kg

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

Skin corrosion/irritation Causes skin irritation.

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.

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

ALLYL CAPROATE (HEXANOATE) FCC < 3600 µg/plate, Strains TA 1535, TA 1537, TA 1538, TA 98 and TA 100 with and without metabolic activation. Vehicle DMSO or Water.
 Result: Not mutagenic.
 Species: Salmonella typhimurium
 Notes: RIFM

Carcinogenicity 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.

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 Very toxic to aquatic life. Harmful to aquatic life with long lasting effects.

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

Bioaccumulative potential

Partition coefficient n-octanol / water (log Kow)

ALLYL CAPROATE (HEXANOATE) FCC 3.18, 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

UN number	UN2810
UN proper shipping name	Toxic liquid, organic, n.o.s. (ALLYL CAPROATE (HEXANOATE) FCC)
Transport hazard class(es)	
Class	6.1(PGIII)
Subsidiary risk	-
Label(s)	6.1
Packing group	III
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Special provisions	IB3, T7, TP1, TP28
Packaging exceptions	153
Packaging non bulk	203
Packaging bulk	241

IATA

UN number	UN2810
UN proper shipping name	Toxic liquid, organic, n.o.s. (ALLYL CAPROATE (HEXANOATE) FCC)
Transport hazard class(es)	
Class	6.1(PGIII)
Subsidiary risk	-
Packing group	III
Environmental hazards	No.
ERG Code	6L
Special precautions for user	Read safety instructions, SDS and emergency procedures before handling.
Other information	
Passenger and cargo aircraft	Allowed.
Cargo aircraft only	Allowed.

IMDG

UN number	UN2810
UN proper shipping name	TOXIC LIQUID, ORGANIC, N.O.S. (ALLYL CAPROATE (HEXANOATE) FCC)
Transport hazard class(es)	
Class	6.1(PGIII)
Subsidiary risk	-
Packing group	III
Environmental hazards	
Marine pollutant	No.
EmS	F-A, S-A
Special precautions for user	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 listed.

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

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)	Yes
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).

IFRA restrictionThere is an IFRA guideline regarding this product. Please visit www.ifraorg.org for the full text of the guideline, or contact Bedoukian Research, Inc. for more information.**16. Other information, including date of preparation or last revision****Issue date** 05-28-2015**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.