



# Safety Data Sheet

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## Section 1: Product & Company Identification

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- 1.1** Product Name: **ALLYL CAPROATE**  
Chemical name: Allyl hexanoate  
Product Number: 9063  
Brand: **Elan Inc.**  
CAS Number: **123-68-2**  
EC Number: **204-642-4**  
FEMA Number: 2032
- 1.2** Recommended use of chemical: Intermediate chemical used in flavor and food application
- 1.3** Supplier details: Elan Inc.  
268 Doremus Avenue  
Newark, NJ 07105  
U.S.A.  
(973) 344-8014  
[jbissonette@elan-chemical.com](mailto:jbissonette@elan-chemical.com)
- 1.4** Emergency telephone: **(800) 424-9300 (Chemtrec)**

## Section 2: Hazard(s) Identification

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- 2.1** Classification of the Substance or mixture: GHS classification in accordance to 29 CFR 1910 (OSHA HCS)

Physical Hazard(s): Flammable liquids: Category 4

Health Hazard(s): Acute toxicity, Oral: Category 3  
Acute toxicity, Dermal: Category 3

Environmental Hazard(s): Acute aquatic toxicity: Category 2  
Chronic aquatic toxicity: Category 2

**2.2** Label Elements:

Pictogram(s):



Signal word:

**Warning**

**Hazard Statement(s):**

**Physical Hazard(s)**

H227 Combustible liquid

**Health Hazard(s)**

H301+H311 Toxic if swallowed or in contact with skin

**Environmental Hazard(s)**

H411 Toxic to aquatic life with long lasting effects

## Precautionary Statement(s):

### **Prevention:**

P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P264	Wash... thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection.

### **Response:**

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor/...
P302+P352	IF ON SKIN: Wash with plenty of water/...
P312	Call a POISON CENTER/doctor/.../if you feel unwell.
P330	Rinse mouth.
P361	Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P370+P378	In case of fire: Use ... to extinguish.
P391	Collect spillage.

### **Storage:**

P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.

### **Disposal:**

P501	Dispose of contents/container to ... your waste control program
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## **2.3 Other Hazards:**

No additional information available

## **Section 3: Composition/Information on Ingredients**

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### **3.1 Substances:**

Identity:	ALLYL CAPROATE		
Synonyms:	Allyl Hexanoate		
CAS Number:	123-68-2		
EC Number:	204-642-4		
Purity:	98.0% min.		
Molecular Formula:	<b>C9 H16 O2</b>	Molecular Weight:	156.2 g/mol

### **3.2 Mixtures:**

Not applicable

## **Section 4: First Aid Measures**

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### **4.1 Description of necessary measures:**

Inhalation Exposure: If inhaled, move to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen. Consult a physician.

Skin Exposure: In case of contact, immediately wash skin with soap and copious amounts of water. Consult a physician.

Eye Exposure: In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes as a precaution.

Oral Exposure: If swallowed; do not induce vomiting. Wash out mouth with water provided person is conscious. Call a physician.

4.2 Most important symptoms/effects, acute and delayed: If you feel unwell, seek medical advice (show the label where possible)

4.3 Indication of immediate medical attention and special treatment, if necessary: If the person is unconscious immediately call 911. Never give anything by mouth to an unconscious person.

## Section 5: Fire Fighting Measures

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5.1 Extinguishing media:

Suitable:	For smaller fires use:	Foam Carbon Dioxide Dry Chemical Powder
	For Larger fires use:	From a distance use very large quantities of misted water (flooding).
Unsuitable:	Unknown	

5.2 Specific hazards arising from the chemical: Emits toxic fumes under fire conditions – carbon oxides.

5.3 Special protective equipment and precautions for fire-fighters: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

5.4 Further information: Use flooding water to cool unopened containers

## Section 6: Accidental Release Measures

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6.1 Personal Precautions, Protective equipment, and emergency procedures: Exercise appropriate precautions to minimize direct contact with skin or eyes and prevent inhalation of vapors, mist or gas. Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in lower areas.

6.2 Environmental precaution: Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up: Contain spillage and ventilate.

Collect with a properly grounded dedicated wet vacuum and place in container for waste disposal (see company waste SOP)

## Section 7: Handling and Storage Procedures

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7.1 Precautions for safe handling: Do not breathe vapor. Avoid contact with eyes, skin and clothing. Avoid prolonged or repeated exposure. No smoking! Avoid any electrostatic charges. Porous material such as rags, paper, insulation, or organic clay may spontaneously combust when wetted with this material. May auto-oxidize with sufficient heat generation to ignite if spread (as a thin film) or absorbed on porous or fibrous material. All equipment used when handling the product must be grounded. Contaminated rags and cloths must be put in fireproof containers for disposal.

7.2 Conditions for safe storage, including any incompatibilities: Keep container tightly closed. Keep away from heat and open flame. Store container(s) in a cool & dry place.

## Section 8: Exposure Controls/Personal Protection

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- 8.1** Control parameters: Contains no substance with occupational limit values.
- 8.2** Appropriate Engineering Controls: Practice proper hygienic and work place safety procedures.
- 8.3** Individual protection measures (PPEs):

Eye Protection:	Chemical Safety goggles
Skin (Hand) Protection:	Chemical resistant gloves
Respiratory protection:	If exposure limits are exceeded or irritation is experienced, NIOSH approved respirator protection should be worn
Other Information:	Wash contaminated clothing before reuse Wash thoroughly after handling When using do not eat, drink or smoke

## Section 9: Physical/Chemical Properties

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Appearance:	colorless to pale yellow liquid
Odor:	N/A
Odor Threshold:	N/A
pH:	13.72
Melting point/freezing point:	N/A °F
Initial Boiling Point and Boiling:	75-76 °C
Flash Point:	151.0 °F 66.1 °C
Evaporation Rate:	N/A
Flammability (solid, gas):	N/A
Upper.lower flammability or explosive limits:	1.9-11 %
Vapor pressure:	0.678
Vapor Density:	N/A
Relative Density:	0.884 - 0.89 g/cm <sup>3</sup>
Refractive index:	1.422-1.426
Solubility (ies):	N/A
Partition coefficient: n-octanol/water:	N/A
Auto-ignition Temperature:	824 °F 440 °C
Decomposition Temperature:	N/A
Viscosity:	N/A

## Section 10: Stability and Reactivity

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- 10.1** Reactivity: no data available
- 10.2** Chemical Stability: Stable under recommended storage conditions.
- 10.3** Possibility of hazardous reactions: Vapors may form explosive mixture with air.
- 10.4** Conditions to avoid: Heat, flames and sparks. Extremes of temperature and direct sunlight.
- 10.5** Incompatible material(s): Oxidizing agents.
- 10.6** Hazardous Decomposition Products: no data available

## Section 11: Toxicological Information

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**11.1** Information on the likely routes of exposure:

Inhalation:	no data available
Ingestion:	no data available
Skin Contact:	May cause skin irritation
Skin Absorption:	no data available
Eye Contact:	may cause serious eye irritation

- 11.2** Symptoms related to the physical, chemical and toxicological characteristics: Basic symptoms include, but are not exclusive, irritation, nausea, unconsciousness (consult specialist or Chemtrec).

11.3 Delayed and immediate effects and also chronic effects from short and long term exposure: Consult physician, specialist and/or Chemtrec.

11.4 Numerical measures of toxicity (acute estimates): To the best of our knowledge, the toxicological properties are the following:

Oral: rat LD50: 218 mg/kg  
Dermal: rabbit LD50: 300 mg/kg  
Inhalation: no data available

## Section 12: Ecological Information

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12.1 Ecotoxicity (aquatic and terrestrial):

Toxicity to fish: LC50 - Pimephales promelas (fathead minnow) - 2.0 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna (Water flea) - 2 mg/l - 48 h

12.2 Persistence and degradability: May not be readily biodegradable.

12.3 Bioaccumulative potential: no data available

12.4 Mobility in soil: no data available

12.5 Other adverse effects: no data available

## Section 13: Disposal Considerations

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Disposal Instructions: Do not discharge into drains, water courses or onto the ground. 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 and international regulations.

Local disposal regulations: Dispose in accordance with all applicable regulations.

Hazardous waste code: Not established.

Waste from residues/unused products: Empty containers or liners may retain some product residues. This material and its products container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging: Empty containers should be taken to an approved waste handling site for recycling or disposal. Since emptied containers may retain product residue, follow label warnings even after container is empty.

## Section 14: Transportation Information

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### DOT (US)

UN#: 2810  
Proper Shipping Name: Toxic liquid, organic, n.o.s.  
Class: 6.1  
Packing Group: III

### IMDG

UN#: 2810  
Proper Shipping Name: Toxic liquid, organic, n.o.s.  
Class: 6.1  
Packing Group: III

### IATA

UN#: 2810  
Proper Shipping Name: Toxic liquid, organic, n.o.s.  
Class: 6.1

## Section 15: Regulatory Information

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### SARA 302 Components

Not subject to reporting requirements of SARA Title III, section 302.

### SARA 313 Components

Not subject to reporting requirements of SARA Title III, section 313.

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

### Massachusetts Right to Know Components

Allyl hexanoate

CAS#: 123-68-2

Revision Date:

### Pennsylvania Right to Know Components

Allyl hexanoate

CAS#: 123-68-2

Revision Date:

### New Jersey Right to Know Components

Allyl hexanoate

CAS#: 123-68-2

Revision Date:

### California Prop. 65 Components

not listed

## Section 16: Other Information

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### Classification according to EU Directives 67/548/EEC or 1999/45/EC

#### Symbol(s):

T N

Toxic. Dangerous for the environment.

#### R - phrase(s):

R: 22 24 51/53

Harmful if swallowed. Toxic in contact with skin. Toxic to aquatic organisms, may cause long term adverse effects in the aquatic environment.

#### S - phrase(s):

S: 36/37 45 61

Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical attention immediately. Avoid release to the environment.

#### HMIS Rating

Health hazard: 2  
 Chronic Health hazard:  
 Flammability: 2  
 Physical hazard: 0

#### NFPA Rating

Health hazard: 2  
 Fire hazard: 2  
 Reactivity hazard: 0

**FEMA GRAS™ (Generally Recognized As Safe) status for the use of a flavor ingredient in food only stipulates current regulatory acceptability for oral ingestion as a food item and does not provide regulatory authority and/or acceptability in the U.S for the use of the flavor ingredient in devices which cause the flavorant to be inhaled.**

**Elan, Inc. does not represent or suggest that this flavor ingredient is safe for use in E-cigarettes.**

*This safety data sheet is intended to meet the specific requirements of GHS and should be used accordingly. While the information has been obtained from sources believed to be accurate and reliable, no warranty, expressed or implied, can be made with regard to its completeness, correctness or accuracy. Any users or handlers of this product who are not under the direct control of Elan Inc. are responsible for evaluating this information in light of their particular situation and are responsible for all losses, damages or expenses that result while this material*

is under their control. It is also the responsibility of the users and handlers to observe any and all laws and regulations (Global, Federal, State and Local) concerning the transportation, use, handling, storage and disposal of this product.

1. Globally Harmonized System of Classification and Labelling of Chemicals (GHS) Sixth revised edition, United Nations, 2015.
2. ISO 11014:2009 Safety data sheet for chemical products -- Content and order of sections.
3. American National Standard for Hazardous Industrial Chemicals-MSDS Preparation (ANSI Z400.1/Z129.1-2010)
4. U.S. DOL, OSHA, 29 CFR 1910.1200, HAZCOM.