



# Safety Data Sheet

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## Section 1: Product & Company Identification

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- 1.1 Product Name:** **ISOBUTYL PHENYLACETATE**  
**Chemical name:** Isobutyl phenylacetate  
**Product Number:** 9089  
**Brand:** **Elan Inc.**  
**CAS Number:** **102-13-6**  
**EC Number:** **203-007-9**  
**FEMA Number:** 2210
- 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  
[qualityassurance@elan-chemical.com](mailto:qualityassurance@elan-chemical.com)
- 1.4 Emergency telephone:** **(800) 424-9300 (Chemtreec)**

## 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):** None

**Health Hazard(s):** Skin irritation: Category 2  
Eye irritation: Category 2A  
Specific target organ toxicity - single exposure: Category 3

**Environmental Hazard(s):** None

**2.2 Label Elements:**

**Pictogram(s):** 

**Signal word:** **Warning**

**Hazard Statement(s):**

**Physical Hazard(s)**

N/A N/A

**Health Hazard(s)**

H315 Causes skin irritation  
H319 Causes serious eye irritation  
H335 May cause respiratory irritation

## Environmental Hazard(s)

N/A

N/A

## Precautionary Statement(s):

### Prevention:

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P264 Wash... thoroughly after handling.  
P271 Use only outdoors or in well-ventilated area.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.

### Response:

P312 Call a POISON CENTER/doctor/.../if you feel unwell.  
P321 Specific treatment (see ... on this label).  
P362 Take off contaminated clothing.  
P302+P352 IF ON SKIN: Wash with plenty of water/...  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P332+P313 If skin irritation occurs: Get medical advice/attention.  
P337+P313 If eye irritation persists: Get medical advice/attention.

### Storage:

P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

### Disposal:

P501 Dispose of contents/container to ... your waste control program

## 2.3 Other Hazards:

No additional information available

## Section 3: Composition/Information on Ingredients

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### 3.1 Substances:

Identity:	Isobutyl phenylacetate		
Synonyms:	2-methylpropyl 2-phenylacetate		
CAS Number:	102-13-6		
EC Number:	203-007-9		
Purity:	98.0% min.		
Molecular Formula:	<b>C<sub>12</sub>H<sub>16</sub>O<sub>2</sub></b>	Molecular Weight:	192.26 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 liquid
Odor:	N/A
Odor Threshold:	N/A
pH:	N/A
Melting point/freezing point:	N/A
Initial Boiling Point and Boiling:	253 °C
Flash Point:	235.0 °F 113.0 °C
Evaporation Rate:	N/A
Flammability (solid, gas):	N/A
Upper.lower flammability or explosive limits:	N/A %
Vapor pressure:	N/A
Vapor Density:	N/A
Relative Density:	0.984 - 0.98 g/cm <sup>3</sup>
Refractive index:	1.486-1.488
Solubility (ies):	N/A
Partition coefficient: n-octanol/water:	N/A
Auto-ignition Temperature:	N/A °F N/A °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: no data available
- 10.4 Conditions to avoid: no data available
- 10.5 Incompatible material(s): Oxidizing agents. Acids and Bases
- 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: no data available  
Skin Absorption: no data available  
Eye Contact: no data available

**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: >5,000 mg/kg  
Dermal: rabbit LD50: >5,000 mg/kg  
Inhalation: no data available

## Section 12: Ecological Information

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**12.1** Ecotoxicity (aquatic and terrestrial): no data available  
**12.2** Persistence and degradability: no data available  
**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)

not dangerous goods

### IMDG

not dangerous goods

### IATA

not dangerous goods

## 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

Acute Health Hazard

### Massachusetts Right to Know Components

Isobutyl phenylacetate CAS#: 102-13-6 Revision Date: 4-24-1993

### Pennsylvania Right to Know Components

Isobutyl phenylacetate CAS#: 102-13-6 Revision Date: 4-24-1993

### New Jersey Right to Know Components

Isobutyl phenylacetate CAS#: 102-13-6 Revision Date: 4-24-1993

### 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):

Xi Irritant

#### R - phrase(s):

R: 36/37/38

#### S - phrase(s):

S: 26 36

#### HMIS Rating

Health hazard: 2  
Chronic Health hazard:  
Flammability: 1  
Physical hazard: 0

#### NFPA Rating

Health hazard: 2  
Fire hazard: 1  
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) Eighth revised edition, United Nations, 2019.
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.
5. Regulation (EC) No. 1272/2008