SECTION 1: Identification

1.1. Identification

Product name: ALLYL PENTAFLUOROBENZENE
Product code: ENEA0378
Product form: Substance
Physical state: Liquid
Formula: C9H5F5
Synonyms: 3-(PENTAFLUOROPHENYL)PROPENE BENZENE, PENTAFLUORO-2-PROPENYL-
Chemical family: FLUORONATED ORGANIC

1.2. Recommended use and restrictions on use

Recommended use: Chemical intermediate

1.3. Supplier

GELEST, INC.
11 East Steel Road
Morrisville, PA 19067
USA
T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST
info@gelest.com - www.gelest.com

1.4. Emergency telephone number

Emergency number: CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification
Flammable liquids Category 3 H226 Flammable liquid and vapor
Skin corrosion/irritation Category 2 H315 Causes skin irritation
Serious eye damage/eye irritation Category 2 H319 Causes serious eye irritation
Full text of H statements: see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling
Hazard pictograms (GHS US): ☢️ ⚠️

Signal word (GHS US): Warning
Hazard statements (GHS US): H26 Flammable liquid and vapor
H315 Causes skin irritation
H319 Causes serious eye irritation

Precautionary statements (GHS US): P280 Wear protective gloves/protective clothing/eye protection/face protection.
P210 Keep away from heat, open flames, sparks. No smoking.
P233 Keep container tightly closed.
P240 Ground/Bond container and receiving equipment.
P241 Use explosion-proof electrical equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P264 Wash hands thoroughly after handling.
P303+P361+P353 If on skin (or hair): take off immediately all contaminated clothing, rinse skin with water/shower.
P332+P335 If skin irritation occurs: Get medical advice/attention.
P335 If skin irritation persists: Get medical advice/attention.
P321 Specific treatment (see first aid instructions on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P370+P378 If eye irritation persists: Get medical advice/attention.
P403+P235 Keep in a cool place.
P501 Dispose of contents/container to licensed waste disposal facility.
2.3. Hazards not otherwise classified (HNOC)

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

<table>
<thead>
<tr>
<th>Name</th>
<th>Product identifier</th>
<th>%</th>
<th>GHS-US classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Allylpentafluorobenzene</td>
<td>(CAS-No.) 1736-60-3</td>
<td>95 - 100</td>
<td>Flam. Liq. 3, H226</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Skin Irrit. 2, H315</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Eye Irrit. 2A, H319</td>
</tr>
</tbody>
</table>

Full text of hazard classes and H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general: Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label.

First-aid measures after inhalation: Remove victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact: Wash with plenty of soap and water. Get medical advice/attention.

First-aid measures after eye contact: Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion: Never give anything by mouth to an unconscious person. Get medical advice/attention.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects after inhalation: May cause irritation to the respiratory tract.

Symptoms/effects after skin contact: Causes skin irritation.

Symptoms/effects after eye contact: Causes serious eye irritation.

Symptoms/effects after ingestion: No information available.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media


Unsuitable extinguishing media: None known.

5.2. Specific hazards arising from the chemical

Fire hazard: Flammable liquid and vapor. Irritating fumes and acid vapors may develop when material is exposed to elevated temperatures or open flame.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions: Exercise caution when fighting any chemical fire. Use water spray or fog for cooling exposed containers.

Protection during firefighting: Do not enter fire area without proper protective equipment, including respiratory protection. Avoid all eye and skin contact and do not breathe vapor and mist.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures: Eliminate ignition sources. Use special care to avoid static electric charges.

6.1.1. For non-emergency personnel

Protective equipment: Wear protective equipment as described in Section 8.

Emergency procedures: Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment: Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: “Exposure controls/personal protection”.
6.2. Environmental precautions
Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up
For containment: Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.
Methods for cleaning up: Clean up any spills as soon as possible, using an absorbent material to collect it. Use only non-sparking tools.

6.4. Reference to other sections
See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling
Additional hazards when processed: Handle empty containers with care because residual vapors are flammable. Keep away from heat, open flames, sparks. - No smoking.
Precautions for safe handling: Avoid all eye and skin contact and do not breathe vapor and mist. Ground/bond container and receiving equipment. Provide good ventilation in process area to prevent accumulation of vapors. Take precautionary measures against static discharge. Use only non-sparking tools.
Hygiene measures: Wash contaminated clothing before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities
Technical measures: Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.
Storage conditions: Keep container tightly closed. Keep in a cool place.
Incompatible materials: Oxidizing agent.
Storage area: Store in a well-ventilated place. Store away from heat.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters
No additional information available

8.2. Appropriate engineering controls
Appropriate engineering controls: Provide local exhaust or general room ventilation.

8.3. Individual protection measures/Personal protective equipment
Personal protective equipment:
Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

Hand protection:
Neoprene or nitrile rubber gloves

Eye protection:
Chemical goggles. Contact lenses should not be worn

Skin and body protection:
Wear suitable protective clothing

Respiratory protection:
Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified organic vapor (black cartridge) respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties
Physical state: Liquid
Appearance: Clear liquid.
Molecular mass: 208.13 g/mol
Color: Straw.
Odor: No data available
Odor threshold: No data available
Refractive index: 1.427
**ALLYL PENTAFLUOROBENZENE**

**Safety Data Sheet**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative evaporation rate (butyl acetate=1)</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>Melting point</td>
<td>-64 °C</td>
</tr>
<tr>
<td>Freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Boiling point</td>
<td>148 - 149 °C</td>
</tr>
<tr>
<td>Flash point</td>
<td>43 °C</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>Flammable liquid and vapor</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>6 mm Hg @ 25°C</td>
</tr>
<tr>
<td>Relative vapor density at 20 °C</td>
<td>&gt; 1</td>
</tr>
<tr>
<td>Relative density</td>
<td>1.36</td>
</tr>
<tr>
<td>% Volatiles</td>
<td>&lt; 3 %</td>
</tr>
<tr>
<td>Solubility</td>
<td>Insoluble in water.</td>
</tr>
<tr>
<td>Log Pow</td>
<td>No data available</td>
</tr>
<tr>
<td>Log Kow</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity, kinematic</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity, dynamic</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosion limits</td>
<td>No data available</td>
</tr>
</tbody>
</table>

### 9.2. Other information

No additional information available

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

No additional information available

#### 10.2. Chemical stability

Stable.

#### 10.3. Possibility of hazardous reactions

No additional information available

#### 10.4. Conditions to avoid

Heat. Sparks. Open flame.

#### 10.5. Incompatible materials

Oxidizing agent.

#### 10.6. Hazardous decomposition products

Organic acid vapors.

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

<table>
<thead>
<tr>
<th>Effect</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute toxicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Skin corrosion/irritation</td>
<td>Causes skin irritation.</td>
</tr>
<tr>
<td>Serious eye damage/irritation</td>
<td>Causes serious eye irritation.</td>
</tr>
<tr>
<td>Respiratory or skin sensitization</td>
<td>Not classified</td>
</tr>
<tr>
<td>Germ cell mutagenicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Reproductive toxicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Specific target organ toxicity – single exposure</td>
<td>Not classified</td>
</tr>
<tr>
<td>Specific target organ toxicity – repeated exposure</td>
<td>Not classified</td>
</tr>
<tr>
<td>Aspiration hazard</td>
<td>Not classified</td>
</tr>
<tr>
<td>Symptoms/effects after inhalation</td>
<td>May cause irritation to the respiratory tract.</td>
</tr>
<tr>
<td>Symptoms/effects after skin contact</td>
<td>Causes skin irritation.</td>
</tr>
</tbody>
</table>

None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen.
### Symptoms/effects after eye contact
- Causes serious eye irritation.

### Symptoms/effects after ingestion
- No information available.

### Reason for classification
- Expert judgment

### SECTION 12: Ecological information

#### 12.1. Toxicity
- No additional information available

#### 12.2. Persistence and degradability
- No additional information available

#### 12.3. Bioaccumulative potential
- No additional information available

#### 12.4. Mobility in soil
- No additional information available

#### 12.5. Other adverse effects
- Other adverse effects: This substance may be hazardous to the environment.
- Effect on the ozone layer: No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Disposal methods
- Sewage disposal recommendations: Do not dispose of waste into sewer.
- Product/Packaging disposal recommendations: Incinerate. Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.
- Additional information: Handle empty containers with care because residual vapors are flammable.
- Ecology - waste materials: Avoid release to the environment.

### SECTION 14: Transport information

#### 14.1. UN number
- UN-No.(DOT): 1993
- DOT NA no.: UN1993

#### 14.2. UN proper shipping name
- Transport document description: UN1993 Flammable liquids, n.o.s. (ALLYLPENTAFLUOROBENZENE), 3, III
- Proper Shipping Name (DOT): Flammable liquids, n.o.s. (ALLYLPENTAFLUOROBENZENE)
- Class (DOT): 3 - Class 3 : Flammable and combustible liquid 49 CFR 173.120
- Packing group (DOT): III - Minor Danger
- Hazard labels (DOT): 3 - Flammable liquid

#### DOT Packaging Non Bulk (49 CFR 173.xxx)
- 203

#### DOT Packaging Bulk (49 CFR 173.xxx)
- 242

#### DOT Packaging Exceptions (49 CFR 173.xxx)
- 150

#### DOT Symbols
- G - Identifies PSN requiring a technical name

#### 14.3. Additional information
- Emergency Response Guide (ERG) Number: 128
- Other information: No supplementary information available.

### Transport by sea
- DOT Vessel Stowage Location: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

### Air transport
- DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27): 60 L
ALLYLPENTAFLUOROBENZENE
Safety Data Sheet

DOT Quantity Limitations Cargo aircraft only (49 : 220 L
CFR 175.75)

SECTION 15: Regulatory information

15.1. US Federal regulations
ALLYLPENTAFLUOROBENZENE (1736-60-3)

TSCA Exemption/Exclusion

CAUTION: This material is supplied for research and development purposes subject to the R&D exemption under TSCA, 40 CFR 720.36, and must meet the requirements of the exemption, including supervision by a "technically qualified individual" as defined by 40 CFR 720.3(ee). The use of this material for "commercial purposes" as defined by 40 CFR 720.3(r) is not permitted in the United States.

Allylpentafluorobenzene (1736-60-3)
Not listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations

CANADA

Allylpentafluorobenzene (1736-60-3)

WHMIS Classification
Class B Division 3 - Combustible Liquid

EU-Regulations

Allylpentafluorobenzene (1736-60-3)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations
No additional information available

15.3. US State regulations
California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

Full text of H-phrases::

H226 Flammable liquid and vapor
H315 Causes skin irritation
H319 Causes serious eye irritation

Abbreviations and acronyms

Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development; GHS: The Globally Harmonized System of Classification and Labelling; APF: Assigned Protection Factor.

Hazard Rating

Health

2 Moderate Hazard - Temporary or minor injury may occur

Flammability

3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F. as well as liquids with flash points between 73 F and 100 F. (Classes IB & IC)

Physical

0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Prepared by safety and environmental affairs.

Date of issue: 02/20/2017 Version: 1.0

SDS US (GHS HazCom 2012) - Custom

According to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Print date: 04/10/2019 EN (English US) SDS ID: ENEA0378
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