



# ALLYLPENTAFLUOROBENZENE

Safety Data Sheet ENEA0378

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## SECTION 1: Identification

### 1.1. Product identifier

Product name : ALLYL PENTAFLUOROBENZENE  
 Product code : ENEA0378  
 Product form : Substance  
 Physical state : Liquid  
 Formula : C<sub>9</sub>H<sub>5</sub>F<sub>5</sub>  
 Synonyms : 3-(PENTAFLUOROPHENYL)PROPENE  
 BENZENE, PENTAFLUORO-2-PROPENYL-  
 Chemical family : FLUORONATED ORGANIC

### 1.2. Recommended use of the chemical and restrictions on use

Recommended use : Chemical intermediate  
 For research use only

### 1.3. Details of the supplier of the safety data sheet

**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](mailto:info@gelest.com) - [www.gelest.com](http://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  
 Skin corrosion/irritation Category 2      H315  
 Serious eye damage/eye irritation Category 2      H319  
 Full text of H statements : see section 16

### 2.2. Label elements

#### GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) : Warning

Hazard statements (GHS-US) : H226 - 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+P313 - If skin irritation occurs: Get medical advice/attention  
 P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
 P337+P313 - If eye 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 - In case of fire: Use water spray or fog, foam, carbon dioxide, dry chemical to

# ALLYLPENTAFLUOROBENZENE

## Safety Data Sheet

extinguish  
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)

No data available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Substance type : Mono-constituent  
Name : ALLYLPENTAFLUOROBENZENE  
CAS No : 1736-60-3

Name	Product identifier	%	GHS-US classification
Allylpentafluorobenzene	(CAS No) 1736-60-3	95 - 100	Flam. Liq. 3, H226 Skin Irrit. 2, H315 Eye Irrit. 2A, H319

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

### 3.2. Mixtures

Not applicable

### 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, both acute and delayed

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

Symptoms/injuries after skin contact : Causes skin irritation.

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

Symptoms/injuries after ingestion : No information available.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Water fog. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media : None known.

### 5.2. Special hazards arising from the substance or mixture

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. Advice for firefighters

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.

# ALLYLPENTAFLUOROBENZENE

## Safety Data Sheet

### 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. Exposure controls

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

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

pH : No data available

Relative evaporation rate (butyl acetate=1) : < 1

Melting point : -64 °C

Freezing point : No data available

Boiling point : 148 - 149 °C

# ALLYLPENTAFLUOROBENZENE

## Safety Data Sheet

Flash point	: 43 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Flammable liquid and vapor
Vapor pressure	: 6 mm Hg @ 25°C
Relative vapor density at 20 °C	: > 1
Relative density	: 1.36
VOC content	: < 3 %
Solubility	: Insoluble in water.
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosion limits	: No data available

### 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

Acute toxicity	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
	None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen.
Reproductive toxicity	: Not classified
STOT-single exposure	: Not classified
STOT-repeated exposure	: Not classified
Aspiration hazard	: Not classified
Symptoms/injuries after inhalation	: May cause irritation to the respiratory tract.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after eye contact	: Causes serious eye irritation.
Symptoms/injuries after ingestion	: No information available.
Reason for classification	: Expert judgment

# ALLYLPENTAFLUOROBENZENE

## Safety Data Sheet

### 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 ozone layer : No additional information available  
Effect on the global warming : No known effects from this product.  
GWPmix comment : No known effects from this product.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment 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  
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L

# ALLYLPENTAFLUOROBENZENE

## Safety Data Sheet

### 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

No additional information available

### 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.

#### HMIS III 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.

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SDS US (GHS HazCom 2012) - Custom

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

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# ALLYLPENTAFLUOROBENZENE

Safety Data Sheet

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