SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form: Substance
Physical state: Liquid
Substance name: ALLYL ISOCYANATE, 96%
Product code: ENEA0090
Formula: C4H5NO
Synonyms: ISOCYANIC ACID, ALLYL ESTER
Chemical family: ESTER

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture: Chemical intermediate
For research and industrial 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 - www.gelest.com

1.4. Emergency telephone number

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

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US):
- Flam. Liq. 3 H226
- Acute Tox. 3 (Oral) H301
- Skin Irrit. 2 H315
- Eye Irrit. 2A H319
- Carc. 1B H350

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US): 

Signal word (GHS-US): Danger
Hazard statements (GHS-US):
- H226 - Flammable liquid and vapor
- H301 - Toxic if swallowed
- H315 - Causes skin irritation
- H319 - Causes serious eye irritation
- H350 - May cause cancer

Precautionary statements (GHS-US):
- P201 - Obtain special instructions before use
- P202 - Do not handle until all safety precautions have been read and understood
- 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
- P330 - Rinse mouth
- P270 - Do not eat, drink or smoke when using this product
- P301+P310 - If swallowed: Immediately call a doctor
- P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing, rinse
ALLYL ISOCYANATE, 96%
Safety Data Sheet

2.3. Other hazards
No additional information available

2.4. Unknown acute toxicity (GHS US)
No data available

SECTION 3: Composition/information on ingredients

3.1. Substance
Substance type: Multi-constituent
Name: ALLYL ISOCYANATE, 96%
CAS No: 1476-23-9

<table>
<thead>
<tr>
<th>Name</th>
<th>Product identifier</th>
<th>%</th>
<th>Classification (GHS-US)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Allyl isocyanate</td>
<td>(CAS No) 1476-23-9</td>
<td>95 - 100</td>
<td>Flam. Liq. 3, H226</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Acute Tox. 3 (Oral), H301</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>
<tr>
<td>Allyl carbamoyl chloride</td>
<td>(CAS No) Not found</td>
<td>1 - 2</td>
<td>Not classified</td>
</tr>
<tr>
<td>Methylene chloride</td>
<td>(CAS No) 75-09-2</td>
<td>0 - 1</td>
<td>Acute Tox. 4 (Oral), H302</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Carc. 1B, H350</td>
</tr>
</tbody>
</table>

3.2. Mixture
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 immediate medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed
Symptoms/injuries after inhalation: No information available.
Symptoms/injuries after skin contact: Causes skin irritation.
Symptoms/injuries after eye contact: Causes serious eye irritation.
Symptoms/injuries after ingestion: Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

4.3. Indication of any immediate medical attention and special treatment needed
No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

5.2. Special hazards arising from the substance or mixture
Fire hazard: Flammable liquid and vapor. Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

5.3. Advice for firefighters
Firefighting instructions: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire.
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: Remove ignition sources. Use special care to avoid static electric charges.

6.1.1. For non-emergency personnel
Emergency procedures: Evacuate unnecessary personnel.

6.1.2. For emergency responders
Protective equipment: Equip cleanup crew with proper protection.

6.2. Environmental precautions
Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up
Methods for cleaning up: Clean up any spills as soon as possible, using an absorbent material to collect it. Sweep or shovel spills into appropriate container for disposal. 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
Precautions for safe handling: Material should be handled in a laboratory hood whenever possible. Avoid all eye and skin contact and do not breathe vapor and mist. 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 hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities
Technical measures: Ground/bond container and receiving equipment. Use explosion-proof electrical equipment.
Storage conditions: Keep container tightly closed. Store in sealed containers less than 5°C.
Incompatible materials: Oxidizing agent.
Storage area: Store in a well-ventilated place. Store away from heat.

7.3. Specific end use(s)
No additional information available

SECTION 8: Exposure controls/personal protection
8.1. Control parameters

<table>
<thead>
<tr>
<th>Substance</th>
<th>USA ACGIH ACGIH TWA (ppm)</th>
<th>USA OSHA OSHA PEL (TWA) (ppm)</th>
<th>USA OSHA OSHA PEL (STEL) (ppm)</th>
<th>USA IDLH US IDLH (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methylene chloride</td>
<td>50 ppm</td>
<td>25 ppm</td>
<td>125 ppm (see 29 CFR 1910.1052)</td>
<td>2300 ppm</td>
</tr>
</tbody>
</table>

8.2. Exposure controls
Appropriate engineering controls: Handle in an enclosing hood with exhaust ventilation. 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.

SECTION 9: Physical and chemical properties
9.1. Information on basic physical and chemical properties
Physical state: Liquid
Appearance: Clear liquid.
Molecular mass: 83.09 g/mol
**Color**: Straw.

**Odor**: Lachrymator. Acrid.

**Odor threshold**: No data available

**Refractive index**: 1.417

**pH**: No data available

**Relative evaporation rate (butyl acetate=1)**: ~ 1

**Melting point**: No data available

**Freezing point**: < 0 °C

**Boiling point**: 87 - 89 °C

**Flash point**: 43 °C

**Auto-ignition temperature**: No data available

**Decomposition temperature**: No data available

**Flammability (solid, gas)**: Flammable liquid and vapor

**Vapor pressure**: > 35 mm Hg @ 25°C

**Relative vapor density at 20 °C**: > 1

**Relative density**: 0.94

**VOC content**: 100 %

**Solubility**: Slightly. Soluble 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

Unstable.

#### 10.3. Possibility of hazardous reactions

No additional information available

#### 10.4. Conditions to avoid

Heat. Open flame. Sparks.

#### 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**: Oral: Toxic if swallowed.

**ALLYL ISOCYANATE, 96% (1476-23-9)**

<table>
<thead>
<tr>
<th>Test</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
<td>178 µl/kg</td>
</tr>
<tr>
<td>ATE US (oral)</td>
<td>173.684 mg/kg body weight</td>
</tr>
</tbody>
</table>

**Allyl isocyanate (1476-23-9)**

<table>
<thead>
<tr>
<th>Test</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
<td>165 mg/kg</td>
</tr>
<tr>
<td>LD50 intravenous mouse</td>
<td>18 mg/kg</td>
</tr>
<tr>
<td>ATE US (oral)</td>
<td>165.000 mg/kg body weight</td>
</tr>
</tbody>
</table>

**Methylene chloride (75-09-2)**

<table>
<thead>
<tr>
<th>Test</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
<td>1600 mg/kg</td>
</tr>
<tr>
<td>LC50 inhalation rat (mg/l)</td>
<td>53 mg/l (Exposure time: 6 h)</td>
</tr>
<tr>
<td>ATE US (oral)</td>
<td>1600.000 mg/kg body weight</td>
</tr>
</tbody>
</table>
Methylene chloride (75-09-2)

ATE US (vapors) 53.000 mg/l/4h
ATE US (dust, mist) 53.000 mg/l/4h

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: May cause cancer.

IARC group: 2A - Probably carcinogenic to humans
National Toxicology Program (NTP) Status: 1 - Evidence of Carcinogenicity, 3 - Reasonably anticipated to be Human Carcinogen

12. Ecological information

12.1. Toxicity

Ecology - water: Very toxic to aquatic life.

Methylene chloride (75-09-2)

LC50 fish 1 140.8 - 277.8 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 1 1532 - 1847 mg/l (Exposure time: 48 h - Species: Daphnia magna [Static])
LC50 fish 2 262 - 855 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])
EC50 Daphnia 2 190 mg/l (Exposure time: 48 h - Species: Daphnia magna)

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Methylene chloride (75-09-2)

BCF fish 1 6.4 - 40
Log Pow 1.25

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Effect on ozone layer: No additional information available
Effect on the global warming: No known ecological damage caused by this product.

13. Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations: Incinerate. Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.
Ecology - waste materials: Avoid release to the environment.

14. Transport information

14.1. UN number

UN-No.(DOT) 3080
DOT NA no. UN3080

14.2. UN proper shipping name

Proper Shipping Name (DOT): Isocyanates, toxic, flammable, n.o.s. (ALLYL ISOCYANATE)

Hazard labels (DOT): 6.1 - Poison 3 - Flammable liquid

DOT Symbols: G - Identifies PSN requiring a technical name

Packing group (DOT): II - Medium Danger

DOT Packaging Exceptions (49 CFR 173.xxx): 153
DOT Packaging Non Bulk (49 CFR 173.xxx): 202
DOT Packaging Bulk (49 CFR 173.xxx): 243

Transport by sea

DOT Vessel Stowage Location: B - (i) The material may be stowed “on deck” or “under deck” on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) “On deck only” on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

DOT Vessel Stowage Other: 25 - Shade from radiant heat, 40 - Stow “clear of living quarters”

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27): 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75): 60 L

SECTION 15: Regulatory information

15.1. US Federal regulations

Allyl isocyanate (1476-23-9)
Listed on the United States TSCA (Toxic Substances Control Act) inventory

Methylene chloride (75-09-2)
Listed on the United States TSCA (Toxic Substances Control Act) inventory
Listed on United States SARA Section 313
SARA Section 313 - Emission Reporting 0.1 %

Allyl carbamoyl chloride (Not found)
Not listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations

Allyl isocyanate (1476-23-9)
Listed on the Canadian NDSL (Non-Domestic Substances List)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ISHL (Industrial Safety and Health Law)

Methylene chloride (75-09-2)
Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on the Canadian DSL (Domestic Substances List)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Japanese Pollutant Release and Transfer Register Law (PRTR Law)
Listed on the Canadian IDL (Ingredient Disclosure List)
Listed on INSQ (Mexican national Inventory of Chemical Substances)
Listed on Turkish inventory of chemical

Allyl carbamoyl chloride (Not found)
15.3. US State regulations

<table>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Methylenecloride (75-09-2)</th>
<th>U.S. - California - Proposition 65 - Carcinogens List</th>
<th>U.S. - California - Proposition 65 - Developmental Toxicity</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Female</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Male</th>
<th>No significance risk level (NSRL)</th>
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</thead>
<tbody>
<tr>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
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</table>

<table>
<thead>
<tr>
<th>Allyl carbamoyl chloride (Not found)</th>
<th>U.S. - California - Proposition 65 - Carcinogens List</th>
<th>U.S. - California - Proposition 65 - Developmental Toxicity</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Female</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Male</th>
<th>No significance risk level (NSRL)</th>
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<td>No</td>
<td>No</td>
<td>No</td>
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</tr>
</tbody>
</table>

SECTION 16: Other Information

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.

Full text of H-phrases:
- Acute Tox. 3 (Oral): Acute toxicity (oral) Category 3
- Acute Tox. 4 (Oral): Acute toxicity (oral) Category 4
- Carc. 1B: Carcinogenicity Category 1B
- Eye Irrit. 2A: Serious eye damage/eye irritation Category 2A
- Flam. Liq. 3: Flammable liquids Category 3
- Skin Irrit. 2: Skin corrosion/irritation Category 2
- H226: Flammable liquid and vapor
- H301: Toxic if swallowed
- H302: Harmful if swallowed
- H315: Causes skin irritation
- H319: Causes serious eye irritation
- H350: May cause cancer

HMIS III Rating

Health: 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
Flammability: 3 Serious Hazard
Physical: 0 Minimal Hazard

Prepared by safety and environmental affairs.
The information contained in this document has been gathered from reference materials and/or Gelest, Inc. test data and is to the best knowledge and belief of Gelest, Inc. accurate and reliable. Such information is offered solely for your consideration, investigation and verification. It is not suggested or guaranteed that the hazard precautions or procedures described are the only ones which exist. Gelest, Inc. makes no warranties, express or implied, with respect to the use of such information and assumes no responsibility therefore. Information on this safety data sheet is not intended to constitute a basis for product specifications.

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