**SECTION 1: Identification**

### 1.1. Identification

Product name: ALLYL ISOCYANATE, 96%

Product code: ENEA0090

Product form: Substance

Physical state: Liquid

Formula: C₄H₅NO

Synonyms: ISOCYANIC ACID, ALLYL ESTER

Chemical family: ESTER

### 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: 1-800-424-9390 (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
- Acute toxicity (oral) Category 3: H301 Toxic if swallowed
- Skin corrosion/irritation Category 2: H315 Causes skin irritation
- Serious eye damage/eye irritation Category 2A: H319 Causes serious eye irritation
- Carcinogenicity Category 1B: H350 May cause cancer

Full text of H statements : see section 16

### 2.2. GHS Label elements, including precautionary statements

**GHS US labeling**

- 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.
  P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
ALLYL ISOCYANATE, 96%
Safety Data Sheet

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>Allyl isocyanate</td>
<td>(CAS-No.) 1476-23-9</td>
<td>95 - 100</td>
<td>Flam. Liq. 3, H226 Skin Irrit. 2, H315 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 Carc. 1B, H350</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 immediate medical advice/attention.

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

Symptoms/effects after inhalation: No information available.
Symptoms/effects after skin contact: Causes skin irritation.
Symptoms/effects after eye contact: Causes serious eye irritation. Lachrymator.
Symptoms/effects after ingestion: Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

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


5.2. Specific hazards arising from the chemical

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. Special protective equipment and precautions for fire-fighters

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 < 5°C.

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

<table>
<thead>
<tr>
<th>Methylene chloride (75-09-2)</th>
<th>ACGIH TWA (ppm)</th>
<th>50 ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACGIH</td>
<td>OSHA PEL (TWA) (ppm)</td>
<td>25 ppm</td>
</tr>
<tr>
<td>OSHA</td>
<td>OSHA PEL (STEL) (ppm)</td>
<td>125 ppm (see 29 CFR 1910.1052)</td>
</tr>
<tr>
<td>IDLH</td>
<td>US IDLH (ppm)</td>
<td>2300 ppm</td>
</tr>
</tbody>
</table>

8.2. Appropriate engineering controls

Appropriate engineering controls: Handle in an enclosing hood with exhaust ventilation. 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.
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
% Volatiles: 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: Not classified

<table>
<thead>
<tr>
<th>ALLYL ISOCYANATE, 96% (1476-23-9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
</tr>
<tr>
<td>ATE US (oral)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Allyl isocyanate (1476-23-9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
</tr>
<tr>
<td>LD50 intravenous mouse</td>
</tr>
</tbody>
</table>
### Allyl isocyanate (1476-23-9)

<table>
<thead>
<tr>
<th>Exposure Route</th>
<th>LD50/oral rat</th>
<th>LC50 inhalation rat (mg/l)</th>
<th>LD50/oral</th>
<th>LC50 inhalation (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATE US (oral)</td>
<td>1600 mg/kg</td>
<td>53 mg/l (Exposure time: 6 h)</td>
<td>1600 mg/kg</td>
<td>53 mg/l/4h</td>
</tr>
<tr>
<td>ATE US (vapors)</td>
<td>53 mg/l/4h</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ATE US (dust, mist)</td>
<td>53 mg/l/4h</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**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.

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

- **IARC group:** 2A - Probably carcinogenic to humans
- **National Toxicology Program (NTP) Status:** 1 - Evidence of Carcinogenicity, 3 - Reasonably anticipated to be Human Carcinogen
- **In OSHA Hazard Communication Carcinogen list:** Yes
- **In OSHA Specifically Regulated Carcinogen list:** Yes

**Reproductive toxicity:** Not classified

**Specific target organ toxicity – single exposure:** Not classified

**Specific target organ toxicity – repeated exposure:** Not classified

**Aspiration hazard:** Not classified

**Symptoms/effects after inhalation:** No information available.

**Symptoms/effects after skin contact:** Causes skin irritation.

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

**Symptoms/effects after ingestion:** Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

**Reason for classification:** Expert judgment

### SECTION 12: Ecological information

#### 12.1. Toxicity

**Ecology - water:** Very toxic to aquatic life.

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

<table>
<thead>
<tr>
<th>Species</th>
<th>EC50 (mg/l)</th>
<th>LC50 (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pimephales promelas (flow-through)</td>
<td>140.8 - 277.8</td>
<td>114.8 - 277.8</td>
</tr>
<tr>
<td>Daphnia magna [Static]</td>
<td>1532 - 1847</td>
<td>262 - 855</td>
</tr>
<tr>
<td>Daphnia magna</td>
<td>190</td>
<td></td>
</tr>
</tbody>
</table>

#### 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

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

<table>
<thead>
<tr>
<th>BCF (fish)</th>
<th>Log Pow</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.4 - 40</td>
<td>1.25</td>
</tr>
</tbody>
</table>

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Other adverse effects

**Effect on the ozone layer:** No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Disposal methods

**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.
Ecology - waste materials: Avoid release to the environment.

SECTION 14: Transport information

14.1. UN number
UN-No. (DOT): 3080
DOT NA no.: UN3080

14.2. UN proper shipping name
Transport document description: UN3080 Isocyanates, toxic, flammable, n.o.s. (ALLYL ISOCYANATE), 6.1 (3), II
Proper Shipping Name (DOT): Isocyanates, toxic, flammable, n.o.s. (ALLYL ISOCYANATE)
Packing group (DOT): II - Medium Danger
Hazard labels (DOT): 6.1 - Poison
3 - Flammable liquid

DOT Packaging Non Bulk (49 CFR 173.xxx): 202
DOT Packaging Bulk (49 CFR 173.xxx): 243
DOT Packaging Exceptions (49 CFR 173.xxx): 153
DOT Symbols: G - Identifies PSN requiring a technical name

14.3. Additional information
Emergency Response Guide (ERG) Number: 155
Other information: No supplementary information available.

Transport by sea
DOT Vessel Stowage Location:
(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 - Protected from sources of heat, 40 - Slow “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
Subject to reporting requirements of 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

CANADA
ALLYL ISOCYANATE, 96%
Safety Data Sheet

**Methylene chloride (75-09-2)**
Listed on the Canadian DSL (Domestic Substances List)

**EU-Regulations**
No additional information available

**Methylene chloride (75-09-2)**
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

**National regulations**

**Allyl isocyanate (1476-23-9)**
Listed on the Canadian NDSL (Non-Domestic Substances List)

**WHMIS Classification**
- Class B Division 2 - Flammable Liquid
- Class D Division 1 Subdivision B - Toxic material causing immediate and serious toxic effects
- Class D Division 2 Subdivision B - Toxic material causing other toxic effects

**Methylene chloride (75-09-2)**
Listed on the Canadian DSL (Domestic Substances List)

**WHMIS Classification**
- Class D Division 1 Subdivision B - Toxic material causing immediate and serious toxic effects
- Class D Division 2 Subdivision A - Very toxic material causing other toxic effects
- Class D Division 2 Subdivision B - Toxic material causing other toxic effects

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**15.3. US State regulations**

**WARNING:** This product can expose you to Methylene chloride, which is known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

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

<table>
<thead>
<tr>
<th>U.S. - California - Proposition 65 - Carcinogens List</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Female</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Male</th>
<th>No significant risk level (NSRL)</th>
<th>Maximum allowable dose level (MADL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>200 µg/day (inhalation)</td>
</tr>
</tbody>
</table>

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

- U.S. - Massachusetts - Right To Know List
- U.S. - New Jersey - Right to Know Hazardous Substance List
- U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List
- U.S. - Pennsylvania - RTK (Right to Know) - Special Hazardous Substances
- U.S. - Pennsylvania - RTK (Right to Know) List

---

**SECTION 16: Other information**

Full text of H-phrases:

- **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

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Print date: 04/10/2019
EN (English US)
SDS ID: ENEA0090
ALLYL ISOCYANATE, 96%  
Safety Data Sheet

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: 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
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: 03/11/2015 Revision date: 03/05/2019 Version: 2.1

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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