



# ALLYL ISOCYANATE, 96%

## Safety Data Sheet ENEAA0090

Date of issue: 03/11/2015

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Version: 2.0

### SECTION 1: Identification

#### 1.1. Identification

Product name : ALLYL ISOCYANATE, 96%  
 Product code : ENEAA0090  
 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](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 | Flammable liquid and vapour   |
| 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

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H226 - Flammable liquid and vapour  
 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, hot surfaces, sparks, open flames and other ignition sources. 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.

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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 skin with water/shower  
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P308+P313 - If exposed or concerned: Get medical advice/attention.  
P332+P313 - If skin irritation occurs: Get medical advice/attention.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P362 - Take off contaminated clothing and wash before reuse.  
P370+P378 - In case of fire: Use water spray or fog, foam, carbon dioxide, dry chemical to extinguish.  
P403+P235 - Keep in a cool place  
P405 - Store locked up.  
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

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

| Name                     | Product identifier  | %        | GHS-US classification   |
|--------------------------|---------------------|----------|---|
| Allyl isocyanate         | (CAS-No.) 1476-23-9 | 95 - 100 | Flam. Liq. 3, H226<br>Acute Tox. 3 (Oral), H301<br>Skin Irrit. 2, H315<br>Eye Irrit. 2A, H319 |
| Allyl carbamoyl chloride | (CAS-No.) Not found | 1 - 2    | Not classified  |
| Methylene chloride       | (CAS-No.) 75-09-2   | 0 - 1    | Acute Tox. 4 (Oral), H302<br>Carc. 1B, H350   |

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.  
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

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

### 5.2. Specific hazards arising from the chemical

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

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### 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 in sealed containers less than 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

| Methylene chloride (75-09-2) |                       |                                |
|------------------------------|-----------------------|--------------------------------|
| ACGIH                        | ACGIH TWA (ppm)       | 50 ppm                         |
| OSHA                         | OSHA PEL (TWA) (ppm)  | 25 ppm                         |
| OSHA                         | OSHA PEL (STEL) (ppm) | 125 ppm (see 29 CFR 1910.1052) |
| IDLH                         | US IDLH (ppm)         | 2300 ppm                       |

### 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

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### 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 vapour |
| 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

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| <b>ALLYL ISOCYANATE, 96% (1476-23-9)</b> |                           |
|--|---------------------------|
| LD50 oral rat                            | 178 µl/kg                 |
| ATE US (oral)                            | 173.684 mg/kg body weight |

| <b>Allyl isocyanate (1476-23-9)</b> |                       |
|-------------------------------------|-----------------------|
| LD50 oral rat                       | 165 mg/kg             |
| LD50 intravenous mouse              | 18 mg/kg              |
| ATE US (oral)                       | 165 mg/kg body weight |

| <b>Methylene chloride (75-09-2)</b> |                              |
|-------------------------------------|------------------------------|
| LD50 oral rat                       | 1600 mg/kg                   |
| LC50 inhalation rat (mg/l)          | 53 mg/l (Exposure time: 6 h) |
| ATE US (oral)                       | 1600 mg/kg body weight       |
| ATE US (vapors)                     | 53 mg/l/4h                   |
| ATE US (dust, mist)                 | 53 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.              |

| <b>Methylene chloride (75-09-2)</b>            |  |
|--|--|
| 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.   |
| 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.

| <b>Methylene chloride (75-09-2)</b> |  |
|-------------------------------------|--|
| 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

| <b>Methylene chloride (75-09-2)</b> |          |
|-------------------------------------|----------|
| 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 the ozone layer : No additional information available

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### 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)
- Class (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132
- 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 : 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  
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

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|  |  |
|--|--|
| <b>Allyl isocyanate (1476-23-9)</b>                        |  |
| Listed on the Canadian NDSL (Non-Domestic Substances List) |  |
| WHMIS Classification                                       | Class B Division 2 - Flammable Liquid<br>Class D Division 1 Subdivision B - Toxic material causing immediate and serious toxic effects<br>Class D Division 2 Subdivision B - Toxic material causing other toxic effects  |
| <b>Methylene chloride (75-09-2)</b>                        |  |
| Listed on the Canadian DSL (Domestic Substances List)      |  |
| WHMIS Classification                                       | Class D Division 1 Subdivision B - Toxic material causing immediate and serious toxic effects<br>Class D Division 2 Subdivision A - Very toxic material causing other toxic effects<br>Class D Division 2 Subdivision B - Toxic material causing other toxic effects |

### EU-Regulations

No additional information available

|  |  |
|--|--|
| <b>Methylene chloride (75-09-2)</b>  |  |
| Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances) |  |

### National regulations

|  |  |
|--|--|
| <b>Allyl isocyanate (1476-23-9)</b>  |  |
| Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)<br>Listed on the Japanese ISHL (Industrial Safety and Health Law)  |  |
| <b>Methylene chloride (75-09-2)</b>  |  |
| Listed on the AICS (Australian Inventory of Chemical Substances)<br>Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)<br>Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory<br>Listed on the Korean ECL (Existing Chemicals List)<br>Listed on NZIoC (New Zealand Inventory of Chemicals)<br>Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)<br>Japanese Pollutant Release and Transfer Register Law (PRTR Law)<br>Listed on the Canadian IDL (Ingredient Disclosure List)<br>Listed on INSQ (Mexican National Inventory of Chemical Substances)<br>Listed on CICR (Turkish Inventory and Control of Chemicals) |  |

### 15.3. US State regulations

|   |   |   |   |                                  |
|---|---|---|---|----------------------------------|
| <b>Methylene chloride (75-09-2)</b>                   |   |   |   |                                  |
| U.S. - California - Proposition 65 - Carcinogens List | U.S. - California - Proposition 65 - Developmental Toxicity | U.S. - California - Proposition 65 - Reproductive Toxicity - Female | U.S. - California - Proposition 65 - Reproductive Toxicity - Male | No significant risk level (NSRL) |
| Yes   | No  | No  | No  | 200 µg/day                       |

|  |  |
|--|--|
| <b>Methylene chloride (75-09-2)</b>  |  |
| U.S. - Massachusetts - Right To Know List<br>U.S. - New Jersey - Right to Know Hazardous Substance List<br>U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List<br>U.S. - Pennsylvania - RTK (Right to Know) - Special Hazardous Substances<br>U.S. - Pennsylvania - RTK (Right to Know) List |  |

## SECTION 16: Other information

Full text of H-phrases::

|      |                               |
|------|-------------------------------|
| H226 | Flammable liquid and vapour   |
| H301 | Toxic if swallowed            |
| H302 | Harmful if swallowed          |
| H315 | Causes skin irritation        |
| H319 | Causes serious eye irritation |
| H350 | May cause cancer              |

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.

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### 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.

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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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