



ALLYL ISOCYANATE, 96%

Safety Data Sheet ENEA0090

Date of issue: 03/11/2015

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Version: 2.0

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) :



GHS02

GHS06

GHS07

GHS08

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

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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. 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

Name	Product identifier	%	Classification (GHS-US)
Allyl isocyanate	(CAS No) 1476-23-9	95 - 100	Flam. Liq. 3, H226 Acute Tox. 3 (Oral), H301 Skin Irrit. 2, H315 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 Carc. 1B, H350

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

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

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.

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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

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

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

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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)	
LD50 oral rat	178 µl/kg
ATE US (oral)	173.684 mg/kg body weight
Allyl isocyanate (1476-23-9)	
LD50 oral rat	165 mg/kg
LD50 intravenous mouse	18 mg/kg
ATE US (oral)	165.000 mg/kg body weight
Methylene chloride (75-09-2)	
LD50 oral rat	1600 mg/kg
LC50 inhalation rat (mg/l)	53 mg/l (Exposure time: 6 h)
ATE US (oral)	1600.000 mg/kg body weight

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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.

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

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/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.
Reason for classification	: Expert judgment

SECTION 12: Ecological information

12.1. Toxicity

Ecology - water	: Very toxic to aquatic life.
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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.

SECTION 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.

SECTION 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)
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Department of Transportation (DOT) Hazard Classes : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132

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

14.3. Additional information

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

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)

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15.3. US State regulations

ALLYL ISOCYANATE, 96%(1476-23-9)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No

Allyl isocyanate (1476-23-9)				
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 significance risk level (NSRL)
No	No	No	No	

Methylene chloride (75-09-2)				
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 significance risk level (NSRL)
Yes	No	No	No	

Allyl carbamoyl chloride (Not found)				
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 significance risk level (NSRL)
No	No	No	No	

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.

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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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