Material Safety Data Sheet (MSDS)

Allyl Isothiocyanate
Prepared by: Triveni Chemicals
Revision Date: 26-August-2025
Version: 1.0

Section 1: Product Identification

- **Product Name:** Allyl Isothiocyanate
- **Chemical Formula:** C4H5NS
- **CAS No:** 57-06-7
- **Recommended Use:** Used as a flavoring agent, in pest control, and chemical synthesis.

- **Supplier:**
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Section 2: Hazards Identification

• **Classification (GHS):** Flammable Liquid (Category 3), Acute Toxicity Oral (Category 3), Skin Corrosive (Category 1B), Eye Damage (Category 1).

• **Signal Word:** Danger

• **Hazard Statements:**

- Flammable liquid and vapor
- Toxic if swallowed
- Causes severe skin burns and eye damage
- May cause respiratory irritation

• **Precautionary Statements:**

- Keep away from heat, sparks, open flames, and hot surfaces
- Do not breathe vapors
- Wear protective gloves, protective clothing, and eye/face protection
- Wash hands thoroughly after handling

Section 3: Composition / Information on Ingredients

• **Chemical Name:** Allyl Isothiocyanate

• **Synonyms:** Mustard oil, Volatile mustard oil

- **CAS Number:** 57-06-7
- **Concentration:** >95%

Section 4: First Aid Measures

- **Inhalation:** Remove person to fresh air. Seek immediate medical attention.
- **Skin Contact:** Immediately wash with plenty of soap and water. Remove contaminated clothing. Seek medical advice immediately.
- **Eye Contact:** Rinse cautiously with water for several minutes. Seek immediate medical attention.
- **Ingestion:** Rinse mouth. Do not induce vomiting. Seek immediate medical advice.

Section 5: Fire-Fighting Measures

- **Suitable Extinguishing Media:** Water spray, foam, dry chemical, carbon dioxide (CO2).
- **Specific Hazards:** Vapors may form explosive mixtures with air. Emits toxic fumes of nitrogen oxides, sulfur oxides, and carbon oxides under fire conditions.
- **Protective Equipment:** Firefighters should wear self-contained breathing apparatus and protective clothing.

Section 6: Accidental Release Measures

• **Personal Precautions:** Use personal protective equipment. Avoid inhalation and skin/eye contact. Ensure proper ventilation.

• **Environmental Precautions:** Prevent entry into drains and waterways.

• **Cleanup Methods:** Absorb with inert material (sand, earth). Collect in suitable container for proper disposal.

Section 7: Handling and Storage

• **Handling:** Avoid inhalation of vapors and contact with skin/eyes. Use only in well-ventilated areas. Keep away from ignition sources.

• **Storage:** Store in tightly closed containers in a cool, dry, well-ventilated place. Protect from heat, sparks, and direct sunlight.

Section 8: Exposure Controls / Personal Protection

• **Exposure Limits:** OSHA PEL: 0.02 ppm (8h TWA)

• **Engineering Controls:** Ensure adequate ventilation and local exhaust systems.

• **Personal Protective Equipment:** Gloves, protective goggles, lab coat, respirator if exposure limits are exceeded.

Section 9: Physical and Chemical Properties

- **Appearance:** Colorless to pale yellow liquid
- **Odor:** Pungent, mustard-like odor
- **Boiling Point:** 150-152 °C
- **Flash Point:** 45 °C (closed cup)
- **Solubility:** Slightly soluble in water; soluble in ethanol and organic solvents
- **Molecular Weight:** 99.15 g/mol

Section 10: Stability and Reactivity

- **Stability:** Stable under normal conditions.
- **Incompatible Materials:** Strong oxidizing agents, acids, bases, and reducing agents.
- **Hazardous Decomposition Products:** Carbon oxides, nitrogen oxides, and sulfur oxides under fire conditions.

Section 11: Toxicological Information

- **Routes of Exposure:** Inhalation, ingestion, skin and eye contact.
- **Acute Effects:** Causes severe irritation, burns, and respiratory distress.

• **Chronic Effects:** Prolonged exposure may cause lung damage, gastrointestinal disorders, and dermatitis.

Section 12: Ecological Information

• **Ecotoxicity:** Harmful to aquatic organisms with potential long-term effects.

• **Persistence and Degradability:** May be biodegradable but with potential environmental hazard.

• **Bioaccumulative Potential:** Moderate potential for bioaccumulation.

Section 13: Disposal Considerations

• Dispose of contents/container in accordance with local/regional/national regulations. Avoid release into the environment.

Section 14: Transport Information

• **UN Number:** UN 1545

• **Proper Shipping Name:** Allyl isothiocyanate

• **Hazard Class:** 6.1 (Toxic substances)

• **Packing Group:** II

Section 15: Regulatory Information

• Complies with Indian chemical safety regulations and listed under international chemical inventories (TSCA, EINECS, etc.).

• Classified as hazardous substance as per GHS.

Section 16: Other Information

- **Prepared By:** Triveni Chemicals, Regulatory Affairs Department
- **Disclaimer:** The above information is believed to be correct but does not claim to be exhaustive. Users are responsible for verifying suitability under actual conditions of use. **Triveni chemicals** disclaims any liability for damage resulting from handling or contact.