

## Safety Data Sheet (United States)

3-Cyanophenyl isothiocyanate

**1. Identification**

Product name: 3-Cyanophenyl isothiocyanate  
Catalog#: 9874AD  
IUPAC name: 3-Isothiocyanatobenzonitrile  
Product use restrictions: Only for research and development use by, or directly under the supervision of, a technically qualified individual.  
Company: AK Scientific, Inc.  
30023 Ahern Ave.  
Union City, CA 94587  
Telephone: (510) 429-8835  
Fax: (510) 429-8836  
Website: www.aksci.com  
Emergency contact number: 1-800-633-8253 United States & Canada  
1-801-629-0667 International

**2. Hazard Identification:****GHS Classification (United States)**

Acute toxicity, Oral (Category 4)  
Acute toxicity, Inhalation (Category 4)  
Acute toxicity, Dermal (Category 4)  
Skin corrosion (Category 1B)  
Serious eye damage (Category 1)  
Respiratory sensitisation (Category 1)  
Skin sensitisation (Category 1)

**Pictogram(s)****Signal word:**

Danger

**Hazard statement(s)**

H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled.  
H314 Causes severe skin burns and eye damage.  
H317 May cause an allergic skin reaction.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

**Precautionary statement(s):**

P260 Do not breathe dust/fume/gas/mist/vapors/spray.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P285 In case of inadequate ventilation wear respiratory protection.  
P301+P312 IF SWALLOWED: Call a poison center or doctor if you feel unwell.  
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.  
P304+P340 IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses,

-	if present and easy to do. Continue rinsing.
P310	Immediately call a poison center or doctor.
P322	Specific measures (see supplemental first aid instructions on this label).
P333+P313	If skin irritation or rash occurs: Get medical advice/attention.
P363	Wash contaminated clothing before reuse.
P405	Store locked up.
P501	Dispose of contents/container to an approved waste disposal plant.

**Hazards not otherwise classified (HNOC) or not covered by GHS:**

Lachrymator

**3. Composition/Information on Ingredients**

Synonyms:	Not available.
CAS#:	3125-78-8
Purity:	98% (GC)
EC:	Not available.

**4. First Aid Measures**

**General Information:** Immediately remove any clothing contaminated by the product. Move out of dangerous area. Consult a physician and show this safety data sheet.

**Inhalation:** Move person to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Obtain medical aid.

**Skin contact:** Immediately flush skin with running water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Obtain medical aid immediately.

**Eye contact:** Immediately flush open eyes with running water for at least 15 minutes. Obtain medical aid immediately.

**Ingestion:** Do NOT induce vomiting without medical advice. Rinse mouth with water. Never administer anything by mouth to an unconscious person. Obtain medical aid immediately.

**Most important symptoms and effects, both acute and delayed:** No further information available. Please see sections 2 and 11.

**Indication of any immediate medical attention and special treatment needed:** No further information available.

**5. Fire Fighting Measures**

**Suitable extinguishing media:** Use water spray, dry chemical, carbon dioxide, or chemical foam.

**Specific hazards arising from the chemical:** Carbon oxides, Nitrogen oxides, Sulfur oxides.

**Advice for firefighters:** As in any fire, wear a NIOSH-approved or equivalent, pressure-demand, self-contained breathing apparatus and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion.

**6. Accidental Release Measures**

**Personal precautions, protective equipment and emergency procedures:** Wear protective equipment and keep unprotected personnel away. Ensure adequate ventilation. Remove all sources of ignition. Prevent further leak or spill if safe to do so. For personal protective equipment, please refer to section 8.

**Environmental precautions:** Do not let product enter drains, other waterways, or soil.

**Methods and materials for containment and cleaning up:** Prevent further leak or spill if safe to do so. Vacuum, sweep up, or absorb with inert material and place into a suitable disposal container.

Consult local regulations for disposal. See section 13 for further disposal information.

## 7. Handling and Storage

**Precautions for safe handling:** Avoid contact with skin, eyes, and personal clothing. Wash hands thoroughly after handling. Avoid breathing fumes. Use only with adequate ventilation. Wear suitable protective clothing, gloves, and eye/face protection. Keep away from sources of ignition. Minimize dust generation and accumulation. Keep container tightly closed. Open and handle container with care. Do not eat, drink, or smoke while handling.

**Conditions for safe storage, including any incompatibilities:** Store in a tightly-closed container when not in use. Store in a cool, dry, well-ventilated area away from incompatible substances. Keep away from sources of ignition. Store long-term at 2-8°C.

## 8. Exposure Controls/Personal Protection

### Exposure limits:

OSHA PEL: Not available.  
NIOSH REL: Not available.  
ACGIH TLV: Not available.

**Appropriate engineering controls:** Avoid contact with skin, eyes, and clothing. Wash hands before breaks and immediately after handling the product. Facilities storing or utilizing this material should be equipped with an eyewash fountain. Use adequate general and local exhaust ventilation to keep airborne concentrations low.

### Personal protection

**Eyes:** Based on an evaluation of the eye or face hazards present, wear chemical splash-resistant safety glasses or goggles with side protection. A face shield may be appropriate in some workplaces. Use eyewear tested and approved under appropriate government standards such as OSHA 29 CFR 1910.133 or EU EN166.

**Hands:** Wear gloves selected based on an evaluation of the possible hazards to hands and skin, the duration of use, the physical conditions of the workplace, and the chemical resistance and physical properties of the glove material.

**Skin and body:** Protective clothing must be selected based on the hazards present in the workplace, the physical environment, the duration of exposure, and other factors. No fabric can provide protection against all potential hazards; therefore it is important to select the appropriate protective clothing for each specific hazard. At the minimum, wear a laboratory coat and close-toed footwear.

**Respiratory:** Respirators are not a substitute for accepted engineering control measures such as enclosure or confinement of the operation, general and local ventilation, and substitution of less toxic materials. When respiratory personal protective equipment is appropriate based on an assessment of respiratory hazards in the workplace, use a NIOSH- or CEN-certified respirator.

## 9. Physical and Chemical Properties

Physical State:	Solid
Molecular Formula:	C8H4N2S
Molecular Weight:	160.2
Odor:	Not available.
pH:	Not available.
Boiling Point Range:	Not available.
Freezing/Melting Point:	64-66°C
Flash Point:	Not available.
Evaporation Rate:	Not available.
Flammability(solid,gas):	Please see section 2.
Explosive limits:	Not available.

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Vapor Pressure:	Not available.
Vapor Density:	Not available.
Solubility:	Not available.
Relative Density:	Not available.
Refractive Index:	Not available.
Volatility:	Not available.
Auto-ignition Temperature:	Not available.
Decomposition Temperature:	Not available.
Partition Coefficient:	Not available.

**10. Stability and Reactivity**

Reactivity:	Not available.
Chemical stability:	Stable under recommended temperatures and pressures.
Possibility of hazardous reactions:	Not available.
Conditions to avoid:	Dust generation.
Incompatible materials:	Strong oxidizing agents.
Hazardous decomposition products:	Carbon oxides, Nitrogen oxides, Sulfur oxides.

**11. Toxicological Information**

RTECS#	Not available.
Acute toxicity:	Not available.
Routes of exposure:	Inhalation, eye contact, skin contact, ingestion.
Symptoms related to the physical, chemical and toxicological characteristics:	Skin contact may result in inflammation characterized by itching, scaling, reddening, blistering, pain or dryness. Eye contact may result in redness, pain or severe eye damage. Inhalation may cause irritation of the lungs and respiratory system. Overexposure may result in serious illness or death.

**Carcinogenicity**

IARC:	Not classified.
NTP:	Not listed.
OSHA:	Not listed.
Acute toxic effects:	Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

**12. Ecological Information**

Ecotoxicity:	Not available.
Persistence and degradability:	Not available.
Bioaccumulative potential:	Not available.
Mobility in soil:	Not available.
Other adverse effects:	Not available.

**13. Disposal Considerations**

Disposal of waste:	Chemical waste generators must determine whether a discarded chemical is classified as hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification. Observe all federal, state and local regulations when disposing of the substance.
Disposal of packaging:	Do not reuse containers. Dispose of as unused product.

**14. Transportation Information****DOT (United States)**

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UN number: UN1759  
Proper shipping name: Corrosive solids, n.o.s. (3-Cyanophenyl isothiocyanate)  
Transport hazard class: 8;Corrosive  
Packing group: III

**IATA**

UN Number: UN1759  
Proper shipping name: Corrosive solid, n.o.s. (3-Cyanophenyl isothiocyanate)  
Transport hazard class: 8;Corrosive  
Packing group: III

**15. Regulatory Information****TSCA (United States)**

This product is NOT on the EPA Toxic Substance Control Act (TSCA) inventory. The product is supplied solely for use in research and development by or under the supervision of a technically qualified individual as defined in 40 CFR § 720 et seq. The health risks have not been fully determined. Any information that is or becomes available will be supplied on the SDS.

California Proposition 65:	Not Available..	
NFPA Rating:	Health:	3
	Flammability:	0
	Instability:	0

**16. Additional Information**

Version: 4

Revision Date: 04/26/2025

Printed Date: 04/27/2025

*The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall AK Scientific be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if AK Scientific has been advised of the possibility of such damages.*