

# SAFETY DATA SHEET

Revision Date 19-Dec-2025

Revision Number 5

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

## 1. Identification

**Product Name** 3-Cyanophenyl isocyanate

**Cat No. :** AC314180000; AC314180010; AC314180050

**CAS No** 16413-26-6  
**Synonyms** No information available

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

### Details of the supplier of the safety data sheet

#### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

#### **Emergency Telephone Number**

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## 2. Hazard(s) identification

### Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

|  |            |
|--|------------|
| Acute oral toxicity                              | Category 4 |
| Acute dermal toxicity                            | Category 4 |
| Acute Inhalation Toxicity - Dusts and Mists      | Category 4 |
| Skin Corrosion/Irritation                        | Category 2 |
| Serious Eye Damage/Eye Irritation                | Category 2 |
| Respiratory Sensitization                        | Category 1 |
| Specific target organ toxicity (single exposure) | Category 3 |
| Target Organs - Respiratory system.              |            |

### Label Elements

**Signal Word**

Danger

### Hazard Statements

Causes skin irritation  
 Causes serious eye irritation  
 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
 May cause respiratory irritation  
 Harmful if swallowed, in contact with skin or if inhaled



### Precautionary Statements

#### Prevention

Wash face, hands and any exposed skin thoroughly after handling  
 Do not eat, drink or smoke when using this product  
 Wear protective gloves/protective clothing/eye protection/face protection  
 Avoid breathing dust/fume/gas/mist/vapors/spray  
 Use only outdoors or in a well-ventilated area  
 In case of inadequate ventilation wear respiratory protection

#### Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing  
 If experiencing respiratory symptoms: Call a POISON CENTER or doctor

#### Skin

IF ON SKIN: Wash with plenty of soap and water  
 Call a POISON CENTER or doctor if you feel unwell  
 If skin irritation occurs: Get medical advice/attention  
 Take off contaminated clothing

#### Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
 If eye irritation persists: Get medical advice/attention

#### Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
 Rinse mouth

#### Storage

Store in a well-ventilated place. Keep container tightly closed  
 Store locked up

#### Disposal

Dispose of contents/container to an approved waste disposal plant

#### Hazards not otherwise classified (HNOC)

None identified

#### Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

## 3. Composition/information on Ingredients

| Component                | CAS No     | Weight % |
|--------------------------|------------|----------|
| 3-Cyanophenyl isocyanate | 16413-26-6 | <=100    |

## 4. First-aid measures

|  |  |
|--|--|
| <b>Eye Contact</b>                         | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.  |
| <b>Skin Contact</b>                        | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.   |
| <b>Inhalation</b>                          | Remove from exposure, lie down. Remove to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Get medical attention.   |
| <b>Ingestion</b>                           | Clean mouth with water. Get medical attention.   |
| <b>Most important symptoms and effects</b> | May cause allergy or asthma symptoms or breathing difficulties if inhaled. . Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing |
| <b>Notes to Physician</b>                  | Treat symptomatically  |

## 5. Fire-fighting measures

|   |  |
|---|--|
| <b>Suitable Extinguishing Media</b>     | Water spray. Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Chemical foam. |
| <b>Unsuitable Extinguishing Media</b>   | No information available   |
| <b>Flash Point Method -</b>             | No information available<br>No information available                         |
| <b>Autoignition Temperature</b>         | No information available   |
| <b>Explosion Limits</b>                 |  |
| <b>Upper</b>                            | No data available  |
| <b>Lower</b>                            | No data available  |
| <b>Sensitivity to Mechanical Impact</b> | No information available   |
| <b>Sensitivity to Static Discharge</b>  | No information available   |

### Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

### Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

### NFPA

|               |                     |                    |                         |
|---------------|---------------------|--------------------|-------------------------|
| <b>Health</b> | <b>Flammability</b> | <b>Instability</b> | <b>Physical hazards</b> |
| 2             | 0                   | 0                  | N/A                     |

## 6. Accidental release measures

|   |  |
|---|--|
| <b>Personal Precautions</b>                 | Ensure adequate ventilation. Use personal protective equipment as required.                                |
| <b>Environmental Precautions</b>            | See Section 12 for additional Ecological Information.  |
| <b>Methods for Containment and Clean Up</b> | Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment. |

## 7. Handling and Storage

|                 |   |
|-----------------|---|
| <b>Handling</b> | Avoid contact with skin and eyes. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.  |
| <b>Storage.</b> | Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep under nitrogen. Incompatible Materials. Strong oxidizing agents. Strong acids. |

## 8. Exposure controls / personal protection

|   |   |
|---|---|
| <b><u>Exposure Guidelines</u></b>           | This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.   |
| <b>Engineering Measures</b>                 | Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.   |
| <b><u>Personal Protective Equipment</u></b> |   |
| <b>Eye/face Protection</b>                  | Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.   |
| <b>Skin and body protection</b>             | Wear appropriate protective gloves and clothing to prevent skin exposure.   |
| <b>Respiratory Protection</b>               | Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. |
| <b>Recommended Filter type:</b>             | Particulates filter conforming to EN 143.   |
| <b>Hygiene Measures</b>                     | Handle in accordance with good industrial hygiene and safety practice.  |

## 9. Physical and chemical properties

|  |                               |                       |                          |
|--|-------------------------------|-----------------------|--------------------------|
| <b><u>Appearance</u></b>                       |                               |                       |                          |
| <b>Physical State</b>                          | Solid                         |                       |                          |
| <b>Color</b>                                   | Off-white                     |                       |                          |
| <b>Odor</b>                                    | No information available      |                       |                          |
| <b>Odor Threshold</b>                          | No information available      |                       |                          |
| <b><u>Property</u></b>                         | <b><u>Values</u></b>          | <b><u>Remarks</u></b> | <b><u>• Method</u></b>   |
| <b>Melting Point/Range</b>                     | 49 - 54 °C / 120.2 - 129.2 °F |                       |                          |
| <b>Softening Point</b>                         | No data available             |                       |                          |
| <b>Boiling Point/Range</b>                     | No information available      |                       |                          |
| <b>Flash Point</b>                             | No information available      | <b>Method -</b>       | No information available |
| <b>Flammability (liquid)</b>                   | Not applicable                | <b>Solid</b>          |                          |
| <b>Flammability (solid,gas)</b>                | No information available      |                       |                          |
| <b>Explosion Limits</b>                        | No data available             |                       |                          |
| <b>Autoignition Temperature</b>                | No data available             |                       |                          |
| <b>Decomposition Temperature</b>               | No data available             |                       |                          |
| <b>pH</b>                                      | No information available      |                       |                          |
| <b>Viscosity</b>                               | Not applicable                | <b>Solid</b>          |                          |
| <b>Water Solubility</b>                        | No information available      |                       |                          |
| <b>Solubility in other solvents</b>            | No information available      |                       |                          |
| <b>Partition Coefficient (n-octanol/water)</b> |                               |                       |                          |
| <b>Vapor Pressure</b>                          | No data available             |                       |                          |
| <b>Density / Specific Gravity</b>              | No data available             |                       |                          |
| <b>Bulk Density</b>                            | No data available             |                       |                          |
| <b>Vapor Density</b>                           | Not applicable                | <b>Solid</b>          |                          |
| <b>Particle characteristics</b>                | No data available             |                       |                          |
| <b><u>Other Information</u></b>                |                               |                       |                          |
| <b>Molecular Formula</b>                       | C8 H4 N2 O                    |                       |                          |
| <b>Molecular Weight</b>                        | 144.13                        |                       |                          |

Evaporation Rate Not applicable - Solid

## 10. Stability and reactivity

**Reactive Hazard** None known, based on information available

**Stability** Moisture sensitive. Air sensitive.

**Conditions to Avoid** Exposure to air. Incompatible products. Exposure to moist air or water.

**Incompatible Materials** Strong oxidizing agents, Strong acids

**Hazardous Decomposition Products** Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

**Hazardous Polymerization** Hazardous polymerization does not occur.

**Hazardous Reactions** None under normal processing.

## 11. Toxicological information

### Information on expected route of exposure

**Inhalation** Not an expected route of exposure.

**Ingestion** May be harmful if swallowed.

**Eyes** Avoid contact with eyes. Irritating to eyes.

**Skin** May cause irritation. Harmful in contact with skin. Avoid contact with skin.

### Toxicology data for the components

**Toxicologically Synergistic Products** No information available

**(b) skin corrosion/irritation;** Category 2

**(c) serious eye damage/irritation;** Category 2

**(d) respiratory or skin sensitization;**

**Respiratory** Category 1

**Skin** No data available

No information available

**(e) germ cell mutagenicity;** No data available

**(f) carcinogenicity;**

The table below indicates whether each agency has listed any ingredient as a carcinogen

| Component                | CAS No     | IARC       | NTP        | ACGIH      | OSHA       | Mexico     |
|--------------------------|------------|------------|------------|------------|------------|------------|
| 3-Cyanophenyl isocyanate | 16413-26-6 | Not listed |

**(g) reproductive toxicity;** No data available

|  |  |
|--|--|
| <b>(h) STOT-single exposure;</b>                 | Category 3   |
| <b>Results / Target organs</b>                   | Respiratory system.  |
| <b>(i) STOT-repeated exposure;</b>               | No data available  |
| <b>Target Organs</b>                             | No information available.  |
| <b>(j) aspiration hazard;</b>                    | Not applicable<br>Solid  |
| <b>Other Adverse Effects</b>                     | The toxicological properties have not been fully investigated.   |
| <b>Symptoms / effects,both acute and delayed</b> | Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing. |
| <b>Other Adverse Effects</b>                     | The toxicological properties have not been fully investigated.   |
| <b>Endocrine Disrupting Properties</b>           | This product does not contain any known or suspected endocrine disruptors.   |

## 12. Ecological information

### Ecotoxicity

Do not empty into drains.

|                                      |                           |
|--------------------------------------|---------------------------|
| <b>Persistence and Degradability</b> | No information available  |
| <b>Bioaccumulation/ Accumulation</b> | No information available. |
| <b>Mobility</b>                      | No information available. |

## 13. Disposal considerations

|                               |   |
|-------------------------------|---|
| <b>Waste Disposal Methods</b> | Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification. |
|-------------------------------|---|

## 14. Transport information

### DOT

|                             |                                |
|-----------------------------|--------------------------------|
| <b>UN-No</b>                | UN3439                         |
| <b>Proper Shipping Name</b> | NITRILES, SOLID, TOXIC, N.O.S. |
| <b>Hazard Class</b>         | 6.1                            |
| <b>Packing Group</b>        | III                            |

### TDG

|                             |                                |
|-----------------------------|--------------------------------|
| <b>UN-No</b>                | UN3439                         |
| <b>Proper Shipping Name</b> | NITRILES, SOLID, TOXIC, N.O.S. |
| <b>Hazard Class</b>         | 6.1                            |
| <b>Packing Group</b>        | III                            |

### IATA

|                             |                                 |
|-----------------------------|---------------------------------|
| <b>UN-No</b>                | UN3439                          |
| <b>Proper Shipping Name</b> | NITRILES, TOXIC, SOLID, N.O.S.* |
| <b>Hazard Class</b>         | 6.1                             |
| <b>Packing Group</b>        | III                             |

### IMDG/IMO

|                             |                                |
|-----------------------------|--------------------------------|
| <b>UN-No</b>                | UN3439                         |
| <b>Proper Shipping Name</b> | NITRILES, SOLID, TOXIC, N.O.S. |
| <b>Hazard Class</b>         | 6.1                            |
| <b>Packing Group</b>        | III                            |

## 15. Regulatory Information

### United States of America Inventory

| Component                | CAS No     | TSCA | TSCA Inventory notification - Active-Inactive | TSCA - EPA Regulatory Flags |
|--------------------------|------------|------|---|-----------------------------|
| 3-Cyanophenyl isocyanate | 16413-26-6 | -    | -   | -                           |

#### Legend:

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)** Not applicable

**TSCA 12(b)** - Notices of Export Not applicable

### International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

| Component                | CAS No     | DSL | NDSL | EINECS | PICCS | ENCS | ISHL | AICS | IECSC | KECL |
|--------------------------|------------|-----|------|--------|-------|------|------|------|-------|------|
| 3-Cyanophenyl isocyanate | 16413-26-6 | -   | -    | -      | -     | -    | -    | -    | -     | -    |

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

### U.S. Federal Regulations

#### **SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

#### **SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA** - Occupational Safety and Health Administration Not applicable

#### **CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations** Not applicable

### **U.S. Department of Transportation**

Reportable Quantity (RQ): N  
 DOT Marine Pollutant N  
 DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

#### Other International Regulations

**Mexico - Grade** No information available

**Authorisation/Restrictions according to EU REACH** Not applicable

| Component                | CAS No     | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|--------------------------|------------|---|---|---|
| 3-Cyanophenyl isocyanate | 16413-26-6 | -   | -   | -   |

#### Safety, health and environmental regulations/legislation specific for the substance or mixture

| Component                | CAS No     | OECD HPV       | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|--------------------------|------------|----------------|------------------------------|---------------------------|--|
| 3-Cyanophenyl isocyanate | 16413-26-6 | Not applicable | Not applicable               | Not applicable            | Not applicable                             |

#### Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

#### Other International Regulations

| Component                | CAS No     | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|--------------------------|------------|---|--|----------------------------|------------------------------------|
| 3-Cyanophenyl isocyanate | 16413-26-6 | Not applicable  | Not applicable   | Not applicable             | Not applicable                     |

## 16. Other Information

**Prepared By** Product stewardship (Regulatory Affairs)  
 Thermo Fisher Scientific  
 email - begel.sdsdesk@thermofisher.com

**Revision Date** 19-Dec-2025

**Print Date** 19-Dec-2025

**Revision Summary** Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

#### Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other

materials or in any process, unless specified in the text

**End of SDS**