

## Chemical Safety Data Sheet MSDS / SDS

**3-Cyanophenyl isocyanate**

Revision Date:2025-02-01 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 3-Cyanophenyl isocyanate  
CBnumber : CB5418752  
CAS : 16413-26-6  
Synonyms : 3-cyanophenyl,3-Cyanophenyl isocyanate

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P405 Store locked up.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

**Hazard statements**

H335 May cause respiratory irritation

H332 Harmful if inhaled

H319 Causes serious eye irritation

H315 Causes skin irritation

H312 Harmful in contact with skin

H302 Harmful if swallowed

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 3-Cyanophenyl isocyanate
Synonyms	: 3-cyanophenyl,3-Cyanophenyl isocyanate
CAS	: 16413-26-6
MF	: C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> O
MW	: 144.13

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NO<sub>x</sub>)

Hydrogen cyanide (hydrocyanic acid) Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

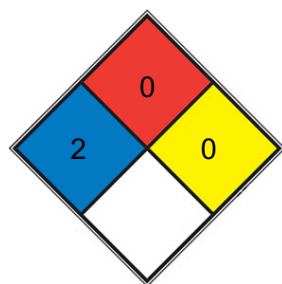
### Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



**HEALTH 2** Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE 0** Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N<sub>2</sub>](#))

**SPEC.**

**HAZ.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### Environmental precautions

Do not let product enter drains.

### Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

## Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

#### Advice on safe handling

Work under hood. Do not inhale substance/mixture.

#### Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed. Dry. Keep locked up or in an area accessible only to qualified or authorized persons.

#### Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: KCL 741 Dermatrif? L

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatril? L

#### Body Protection

protective clothing

#### Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

#### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	yellow crystalline
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 51 - 54 °C - lit.
Initial boiling point and boiling range	123 °C at 16 hPa
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

## SECTION 10: Stability and reactivity

### Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### Possibility of hazardous reactions

No data available

### Conditions to avoid

no information available

### Incompatible materials

Strong oxidizing agents, Strong acids

### Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

Acute toxicity estimate Oral - 500,1 mg/kg (Expert judgment)

Acute toxicity estimate Oral - Expert judgment - 500,1 mg/kg Acute toxicity estimate Inhalation - 4 h - 1,5 mg/l  
(Expert judgment)

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 1,5 mg/l Acute toxicity estimate Dermal - 1.100 mg/kg  
(Expert judgment)

Acute toxicity estimate Dermal - Expert judgment - 1.100 mg/kg

#### Skin corrosion/irritation

Causes skin irritation.

#### Serious eye damage/eye irritation

Causes serious eye irritation.

#### Respiratory or skin sensitization

May cause allergic respiratory and skin reactions

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

No data available

#### Reproductive toxicity

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

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## SECTION 12: Ecological information

### Toxicity

No data available

### Persistence and degradability

No data available

### Bioaccumulative potential

No data available

### Mobility in soil

No data available

### Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### Waste treatment methods

### Product

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### UN number

ADR/RID: - IMDG: - IATA: 3335

## UN proper shipping name

ADR/RID: Not dangerous goods IMDG: Not dangerous goods

IATA: Aviation regulated solid, n.o.s. (3-Isocyanatobenzonitrile)

## Transport hazard class(es)

ADR/RID: - IMDG: - IATA: 9

## Packaging group

ADR/RID: - IMDG: - IATA: III

## Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

## Special precautions for user

No data available

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## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

EC Inventory:Not Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

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## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.