

4-Cyanophenyl isocyanate

sc-232625



The Power to Question

Material Safety Data Sheet

Hazard Alert Code
Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

4-Cyanophenyl isocyanate

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

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EMERGENCY

ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS

C8-H4-N2-O, "4-cyanophenyl isocyanate", 4-cyanophenylisocyanate

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

	Min	Max
Flammability	1	
Toxicity	2	
Body Contact	2	
Reactivity	1	
Chronic	2	

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Contact with acids liberates very toxic gas.
Harmful by inhalation, in contact with skin and if swallowed.
Irritating to eyes, respiratory system and skin.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage to the health of the individual.
- Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide. The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin.
- Aromatic nitriles, unlike aliphatic nitriles, do not appear to liberate cyanide within the body.

EYE

- This material can cause eye irritation and damage in some persons.

SKIN

- Skin contact with the material may be harmful; systemic effects may result following absorption.
- This material can cause inflammation of the skin on contact in some persons.
- The material may accentuate any pre-existing dermatitis condition.
- Open cuts, abraded or irritated skin should not be exposed to this material.
- Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

- Inhalation of dusts, generated by the material, during the course of normal handling, may be harmful.
- The material can cause respiratory irritation in some persons. The body's response to such irritation can cause further lung damage.
- Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.
- The vapor/mist may be highly irritating to the upper respiratory tract and lungs; the response may be severe enough to produce bronchitis and pulmonary edema.

Possible neurological symptoms arising from isocyanate exposure include headache, insomnia, euphoria, ataxia, anxiety neurosis, depression and paranoia.

CHRONIC HEALTH EFFECTS

- Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

There is some evidence that inhaling this product is more likely to cause a sensitization reaction in some persons compared to the general population.

There is limited evidence that, skin contact with this product is more likely to cause a sensitization reaction in some persons compared to the general population.

Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung.

Persons with a history of asthma or other respiratory problems or are known to be sensitised, should not be engaged in any work involving the handling of isocyanates. [CCTRADE-Bayer, APMF].

Chronic exposure to cyanides and certain nitriles may result in interference to iodine uptake by thyroid gland and its consequent enlargement. This occurs following metabolic conversion of the cyanide moiety to thiocyanate.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
4-isocyanatobenzonitrile	40465-45-0	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

- IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.
- Where Medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise

EYE

If this product comes in contact with the eyes

- Wash out immediately with fresh running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN

If skin contact occurs

- Immediately remove all contaminated clothing, including footwear
- Flush skin and hair with running water (and soap if available).

INHALED

- If fumes or combustion products are inhaled remove from contaminated area.
- Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN

- for poisons (where specific treatment regime is absent)

-----BASIC TREATMENT

- Establish a patent airway with suction where necessary.
- Watch for signs of respiratory insufficiency and assist ventilation as necessary.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not Available
Specific Gravity (water=1)	Not Available
Lower Explosive Limit (%)	Not Available

EXTINGUISHING MEDIA

- Small quantities of water in contact with hot liquid may react violently with generation of a large volume of rapidly expanding hot sticky semi-solid foam.
- Presents additional hazard when **FIRE FIGHTING** in a confined space.
- Cooling with flooding quantities of water reduces this risk.
- Water spray or fog may cause frothing and should be used in large quantities.
- Foam.
- Dry chemical powder.

FIRE FIGHTING

- Alert Emergency Responders and tell them location and nature of hazard.
- Wear full body protective clothing with breathing apparatus.

When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 800 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Combustible.

- Moderate fire hazard when exposed to heat or flame.

Combustion products include carbon monoxide (CO), carbon dioxide (CO₂), isocyanates, and minor amounts of, hydrogen cyanide, nitrogen oxides (NO_x), other pyrolysis products typical of burning organic material.

FIRE INCOMPATIBILITY

Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

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Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.
- Use dry clean up procedures and avoid generating dust.
- Place in a suitable, labelled container for waste disposal.

MAJOR SPILLS

For isocyanate spills of less than 40 litres (2 m²)

- Evacuate area from everybody not dealing with the emergency, keep them upwind and prevent further access, remove ignition sources and, if inside building, ventilate area as well as possible.
- Notify supervision and others as necessary.
- Put on personal protective equipment (suitable respiratory protection, face and eye protection, protective suit, gloves and impermeable boots).
- Control source of leakage (where applicable).
- Dike the spill to prevent spreading and to contain additions of decontaminating solution.
- Prevent the material from entering drains.
- Estimate spill pool volume or area.
- Absorb and decontaminate. - Completely cover the spill with wet sand, wet earth, vermiculite or other similar absorbent. - Add neutraliser (for suitable formulations see below) to the adsorbent materials (equal to that of estimated spill pool volume). Intensify contact between spill, absorbent and neutraliser by carefully mixing with a rake and allow to react for 15 minutes
- Shovel absorbent/decontaminant solution mixture into a steel drum.
- Decontaminate surface. - Pour an equal amount of neutraliser solution over contaminated surface. - Scrub

area with a stiff bristle brush, using moderate pressure. - Completely cover decontaminant with vermiculite or other similar absorbent. - After 5 minutes, shovel absorbent/decontamination solution mixture into the same steel drum used above.

- Monitor for residual isocyanate. If surface is decontaminated, proceed to next step. If contamination persists, repeat decontaminate procedure immediately above
- Place loosely covered drum (release of carbon dioxide) outside for at least 72 hours. Label waste-containing drum appropriately. Remove waste materials for incineration.
- Decontaminate and remove personal protective equipment.
- Return to normal operation.
- Conduct accident investigation and consider measures to prevent reoccurrence.

Decontamination

Treat isocyanate spills with sufficient amounts of isocyanate decontaminant preparation ("neutralising fluid"). Isocyanates and polyisocyanates are generally not miscible with water. Liquid surfactants are necessary to allow better dispersion of isocyanate and neutralising fluids/ preparations. Alkaline neutralisers react faster than water/surfactant mixtures alone.

Typically, such a preparation may consist of

Sawdust 20 parts by weight Kieselguhr 40 parts by weight plus a mixture of {ammonia (s.g. 0.880) 8% v/v non-ionic surfactant 2% v/v water 90% v/v}.

Let stand for 24 hours

Three commonly used neutralising fluids each exhibit advantages in different situations.

Formulation A

liquid surfactant 0.2-2%

sodium carbonate 5-10%

water to 100%

Formulation B

liquid surfactant 0.2-2%

concentrated ammonia 3-8%

water to 100%

Formulation C

ethanol, isopropanol or butanol 50%

concentrated ammonia 5%

water to 100%

After application of any of these formulae, let stand for 24 hours.

Formulation B reacts faster than Formulation A. However, ammonia-based neutralisers should be used only under well-ventilated conditions to avoid overexposure to ammonia or if members of the emergency team wear suitable respiratory protection. Formulation C is especially suitable for cleaning of equipment from unreacted isocyanate and neutralizing under freezing conditions. Regard has to be taken to the flammability of the alcoholic solution.

- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

- Do NOT cut, drill, grind or weld such containers.
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

RECOMMENDED STORAGE METHODS

- Lined metal can, Lined metal pail/drum
- Plastic pail

For low viscosity materials

- Drums and jerricans must be of the non-removable head type.

- Where a can is to be used as an inner package, the can must have a screwed enclosure.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- 4-isocyanatobenzonitrile CAS40465-45-0

PERSONAL PROTECTION



RESPIRATOR

- Particulate. (AS/NZS 1716 & 1715, EN 1432000 & 1492001, ANSI Z88 or national equivalent)

EYE

- Safety glasses with side shields.
- Chemical goggles.

HANDS/FEET

NOTE The material may produce skin sensitization in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739, AS/NZS 2161.1 or national equivalent).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374, AS/NZS 2161.10.1 or national equivalent) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

- Isocyanate resistant materials include Teflon, Viton, nitrile rubber and some PVA gloves.
- Protective gloves and overalls should be worn as specified in the appropriate national standard.
- Contaminated garments should be removed promptly and should not be re-used until they have been decontaminated.
- NOTE Natural rubber, neoprene, PVC can be affected by isocyanates

OTHER

- Overalls.
- Eyewash unit.

ENGINEERING CONTROLS

Spraying of material or material in admixture with other components must be carried out in conditions conforming to local state regulations. Local exhaust ventilation with full face air supplied breathing apparatus (hood or helmet type) is normally required.

- Local exhaust ventilation is required where solids are handled as powders or crystals; even when particulates are relatively large, a certain proportion will be powdered by mutual friction.
- Exhaust ventilation should be designed to prevent accumulation and recirculation of particulates in the workplace.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Contact with acids liberates very toxic gas.

State	Divided Solid	Molecular Weight	144.13
Melting Range (°F)	214- 219	Viscosity	Not Applicable
Boiling Range (°F)	Not Applicable	Solubility in water (g/L)	Partly Miscible
Flash Point (°F)	Not Available	pH (1% solution)	Not Applicable
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not Applicable
Autoignition Temp (°F)	Not Available	Vapour Pressure (mmHG)	Negligible
Upper Explosive Limit (%)	Not Available	Specific Gravity (water=1)	Not Available
Lower Explosive Limit (%)	Not Available	Relative Vapor Density (air=1)	Not Applicable
Volatile Component (%vol)	Negligible	Evaporation Rate	Not Applicable

APPEARANCE

Solid; does not mix well with water.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

STORAGE INCOMPATIBILITY

- Avoid reaction with water, alcohols and detergent solutions.
- Isocyanates and thioisocyanates are incompatible with many classes of compounds, reacting exothermically to release toxic gases. Reactions with amines, strong bases, aldehydes, alcohols, alkali metals, ketones, mercaptans, strong oxidisers, hydrides, phenols, and peroxides can cause vigorous releases of heat. Acids and bases initiate polymerisation reactions in these materials.
- Isocyanates easily form adducts with carbodiimides, isothiocyanates, ketenes, or with substrates containing activated CC or CN bonds.
- Some isocyanates react with water to form amines and liberate carbon dioxide. This reaction may also generate large volumes of foam and heat. Foaming in confined spaces may produce pressure in confined spaces or containers. Gas generation may pressurise drums to the point of rupture.
- Do NOT reseal container if contamination is expected
- Open all containers with care
- Base-catalysed reactions of isocyanates with alcohols should be carried out in inert solvents. Such reactions in the absence of solvents often occur with explosive violence,
- Isocyanates will attack and embrittle some plastics and rubbers.
- A range of exothermic decomposition energies for isocyanates is given as 20-30 kJ/mol.
- The relationship between energy of decomposition and processing hazards has been the subject of discussion; it is suggested that values of energy released per unit of mass, rather than on a molar basis (J/g) be used in the assessment.
- For example, in "open vessel processes" (with man-hole size openings, in an industrial setting), substances with exothermic decomposition energies below 500 J/g are unlikely to present a danger, whilst those in "closed vessel processes" (opening is a safety valve or bursting disk) present some danger where the decomposition energy exceeds 150 J/g.

BREThERICK Handbook of Reactive Chemical Hazards, 4th Edition.
For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

4-isocyanatobenzonitrile

TOXICITY AND IRRITATION

4-ISOCYANATOBENZONITRILE

unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

No significant acute toxicological data identified in literature search.

Isocyanate vapors are irritating to the airways and can cause their inflammation, with wheezing, gasping, severe distress, even loss of consciousness and fluid in the lungs. Nervous system symptoms that may occur include headache, sleep disturbance, euphoria, inco-ordination, anxiety, depression and paranoia.

Section 12 - ECOLOGICAL INFORMATION

This material and its container must be disposed of as hazardous waste.

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information

Reactivity characteristic: use EPA hazardous waste number D003 (waste code R).

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

‡ Puncture containers to prevent re-use and bury at an authorized landfill.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

- Recycle wherever possible.
- Consult manufacturer for recycling options or consult Waste Management Authority for disposal if no suitable treatment or disposal facility can be identified.

Section 14 - TRANSPORTATION INFORMATION

DOT:

Symbols:	None	Hazard class or Division:	6.1
Identification Numbers:	UN2206	PG:	III
Label Codes:	6.1	Special provisions:	IB3, T7, TP1, TP13, TP28
Packaging: Exceptions:	153	Packaging: Non-bulk:	203
Packaging: Exceptions:	153	Quantity limitations: Passenger aircraft/rail:	60 L
Quantity Limitations: Cargo aircraft only:	220 L	Vessel stowage: Location:	E
Vessel stowage: Other:	25, 40, 48		

Hazardous materials descriptions and proper shipping names:

Isocyanates, toxic, n.o.s. or Isocyanate solutions, toxic, n.o.s., flash point more than 61 degrees C and boiling point less than 300 degrees C

Air Transport IATA:

ICAO/IATA Class:	6.1	UN/ID Number:	2206
Packing Group:	III	Special provisions:	A3
		Cargo Only	
		Packing Instructions:	663
Maximum Qty/Pack:	220 L	Passenger and Cargo	
Passenger and Cargo		Packing Instructions:	Y642
Maximum Qty/Pack:	60 L	Passenger and Cargo Limited Quantity	
Passenger and Cargo Limited Quantity		Packing Instructions:	655
Maximum Qty/Pack:	2 L		

Shipping Name: ISOCYANATE SOLUTION, TOXIC, N.O.S. *

†(CONTAINS 4-ISOCYANATOBENZONITRILE)

Maritime Transport IMDG:

IMDG Class:	6.1	IMDG Subrisk:	None
UN Number:	2206	Packing Group:	III
EMS Number:	F-A,S-A	Special provisions:	223 274
Limited Quantities:	5 L		

Shipping Name: ISOCYANATES, TOXIC, N.O.S. or ISOCYANATE SOLUTION, TOXIC, N.O.S.(contains 4-isocyanatobenzonitrile)

Section 15 - REGULATORY INFORMATION

4-isocyanatobenzonitrile (CAS: 40465-45-0) is found on the following regulatory lists;

"Canada Non-Domestic Substances List (NDSL)","US Toxic Substances Control Act (TSCA) - Chemical Substance Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

- Cumulative effects may result following exposure*.
- Possible respiratory and skin sensitiser*.

* (limited evidence).

Denmark Advisory list for selfclassification of dangerous substances

Substance	CAS	Suggested codes
4- isocyanatobenzonitrile	40465- 45- 0	R43 Xi; R38

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■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:

www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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