

4-Fluorophenyl isothiocyanate

sc-232730

Material Safety Data Sheet



The Power to Question

Hazard Alert Code Key: **EXTREME** **HIGH** **MODERATE** **LOW**

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

4-Fluorophenyl isothiocyanate

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

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SYNONYMS

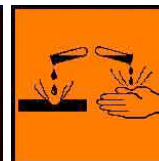
C7-H4-F-S, FC6H4N=C=S, "isothiocyanic acid, p-fluorophenyl ester", "p-fluorophenyl isothiocyanate"

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	3		
Body Contact:	3		
Reactivity:	1		
Chronic:	2		

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



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

Toxic if swallowed.
Causes burns.
Risk of serious damage to eyes.
May cause SENSITISATION by inhalation and skin contact.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- Toxic effects may result from the accidental ingestion of the material; animal experiments indicate that ingestion of less than 40 gram may be fatal or may produce serious damage to the health of the individual.
- The material can produce chemical burns within the oral cavity and gastrointestinal tract following ingestion.

EYE

- The material can produce chemical burns to the eye following direct contact.
Vapors or mists may be extremely irritating.
- If applied to the eyes, this material causes severe eye damage.
- Irritation of the eyes may produce a heavy secretion of tears (lachrymation).

SKIN

- The material can produce chemical burns following direct contact with the skin.
- Skin contact is not thought to produce harmful health effects (as classified using animal models).
Systemic harm, however, has been identified following exposure of animals by at least one other route and the material may still produce health damage following entry through wounds, lesions or abrasions.
- 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.
- Solution of material in moisture on the skin, or perspiration, may markedly increase skin corrosion and accelerate tissue destruction.

INHALED

- If inhaled, this material can irritate the throat and lungs of some persons.
- The material is not thought to produce adverse health effects following inhalation (as classified using animal models).
Nevertheless, adverse effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.
- Inhalation hazard is increased at higher temperatures.
- Inhalation of quantities of liquid mist may be extremely hazardous, even lethal due to spasm, extreme irritation of larynx and bronchi, chemical pneumonitis and pulmonary edema.

CHRONIC HEALTH EFFECTS

- Repeated or prolonged exposure to corrosives may result in the erosion of teeth, inflammatory and ulcerative changes in the mouth and necrosis (rarely) of the jaw. Bronchial irritation, with cough, and frequent attacks of bronchial pneumonia may ensue.
Inhaling this product is more likely to cause a sensitization reaction in some persons compared to the general population.
Skin contact with the material is more likely to cause a sensitization reaction in some persons compared to the general population.
Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

Isothiocyanates have been used as inducers of apoptosis (programmed cell death).

Isothiocyanate-induced apoptosis may suppress the growth of pre-clinical tumours and contribute to the well-established decreased cancer incidence associated with a vegetable-rich diet. Under physiological conditions, isothiocyanates react rapidly with cysteinyl thiol groups to form S-thiocarbamoylcysteine derivatives - which is reversible, and slowly with amino groups to form thioureas. A competing reaction is the hydrolysis of isothiocyanates to corresponding monothiocarbamates and fragmentation to the related amines.

The chemopreventive activity of dietary isothiocyanates has been attributed to the decreased activation and increased conjugation of excretion of carcinogens. Isothiocyanates and their cysteine conjugates inhibited cytochrome P450 isozymes 1A1, 1A2, 2B1 and 2E1. They also induced increased activities of enzymes involved in the detoxification and conjugation of carcinogens for elimination: glutathione S-transferases, quinone reductase, epoxide hydrolase and UDP glucuronosyl transferases. A further feature of the pharmacological activity of dietary isothiocyanates and related S-(N-thiocarbamoyl)cysteine derivatives was their anticancer activity. Inhibition of tumour growth in pre-clinical development by isothiocyanates may contribute to the association of decreased cancer incidence with dietary glucosinolate consumption. Cruciferous vegetables are the major dietary source of naturally occurring thioglucosides or glucosinolates. Glucosinolates are degraded non-enzymatically and enzymatically during food preparation, cooking and chewing.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
4-fluorophenyl isothiocyanate	1544-68-9	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

· For advice, contact a Poisons Information Center or a doctor at once. · Urgent hospital treatment is likely to be needed.

EYE

■ If this product comes in contact with the eyes: · Immediately hold eyelids apart and flush the eye continuously with 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 or hair contact occurs: · Immediately flush body and clothes with large amounts of water, using safety shower if available. · Quickly remove all contaminated clothing, including footwear.

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested. Inhalation of vapors or aerosols (mists, fumes) may cause lung edema. Corrosive substances may cause lung damage (e.g.

NOTES TO PHYSICIAN

■ Treat symptomatically.

for corrosives:

-----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):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	Not available
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

· 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.
 · Slight fire hazard when exposed to heat or flame.
 Combustion products include: carbon dioxide (CO₂), hydrogen fluoride, nitrogen oxides (NO_x), sulfur oxides (SO_x), other pyrolysis products typical of burning organic material.
 May emit corrosive fumes.

FIRE INCOMPATIBILITY

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

PERSONAL PROTECTION

Glasses:
 Safety Glasses.
 Full face- shield.
 Gloves:
 Respirator:
 Type A Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

· Drains for storage or use areas should have retention basins for pH adjustments and dilution of spills before discharge or disposal of

material.

- Check regularly for spills and leaks.
- Clean up all spills immediately.
- Avoid breathing vapors and contact with skin and eyes.

MAJOR SPILLS

- 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

- DO NOT allow clothing wet with material to stay in contact with skin.
- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

- Glass container.
- 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.
- Moisture sensitive.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- 4-fluorophenyl isothiocyanate: CAS:1544-68-9

PERSONAL PROTECTION



RESPIRATOR

- type a filter of sufficient capacity.

EYE

- Chemical goggles.
- Full face shield.

HANDS/FEET

- Wear chemical protective gloves, eg. PVC.
- When handling corrosive liquids, wear trousers or overalls outside of boots, to avoid spills entering boots.

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: such as:

- 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).

- 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) 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) 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.

- Neoprene gloves.

OTHER

- Overalls.
- PVC Apron.

ENGINEERING CONTROLS

- General exhaust is adequate under normal operating conditions. Local exhaust ventilation may be required in special circumstances.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Corrosive.

State	LIQUID	Molecular Weight	153.18
Melting Range (°F)	79- 82	Viscosity	Not Available
Boiling Range (°F)	442	Solubility in water (g/L)	Reacts
Flash Point (°F)	193	pH (1% solution)	Not available
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Not available
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	Not available
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	>1
Volatile Component (%vol)	Not available	Evaporation Rate	Not available

APPEARANCE

Yellow liquid or solid dependent on ambient conditions; hydrolyses in water.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

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

STORAGE INCOMPATIBILITY

- Reacts with mild steel, galvanized steel / zinc producing hydrogen gas which may form an explosive mixture with air.

Segregate from alcohol, water.

Isothiocyanates (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.

- Avoid reaction with oxidizing agents.

- NOTE: May develop pressure in containers; open carefully. Vent periodically.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

4-fluorophenyl isothiocyanate

TOXICITY AND IRRITATION

4-FLUOROPHENYL ISOTHIOCYANATE:

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

TOXICITY	IRRITATION
Intravenous (mouse) LD50: 56 mg/kg	Nil Reported
■ Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's edema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type. Allergic reactions involving the respiratory tract are usually due to interactions between IgE antibodies and allergens and occur rapidly. Allergic potential of the allergen and period of exposure often determine the severity of symptoms. Attention should be paid to atopic diathesis, characterized by increased susceptibility to nasal inflammation, asthma and eczema. Exogenous allergic alveolitis is induced essentially by allergen specific immune-complexes of the IgG type; cell-mediated reactions (T lymphocytes) may be involved. Such allergy is of the delayed type with onset up to four hours following exposure.	

The material may be irritating to the eye, with prolonged contact causing inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.

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.

The material may produce respiratory tract irritation, and result in damage to the lung including reduced lung function.

The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of vesicles, scaling and thickening of the skin.

Section 12 - ECOLOGICAL INFORMATION

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

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
4-fluorophenyl isothiocyanate	HIGH	No Data Available	LOW	MED

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information

Corrosivity characteristic: use EPA hazardous waste number D002 (waste code C)

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. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. 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: 8

Identification Numbers: UN1760 PG: III

Label Codes: 8 Special provisions: IB3, T7, TP1, TP28

Packaging: Exceptions: 154 Packaging: Non- bulk: 203

Packaging: Exceptions: 154 Quantity limitations: 5 L

Passenger aircraft/rail:

Quantity Limitations: Cargo 60 L Vessel stowage: Location: A aircraft only:

Vessel stowage: Other: 40

Hazardous materials descriptions and proper shipping names:

Corrosive liquids, n.o.s.

Air Transport IATA:

UN/ID Number: 1760 Packing Group: III

Special provisions: A3

Cargo Only

Packing Instructions: 60 L Maximum Qty/Pack: 856

Passenger and Cargo Passenger and Cargo

Packing Instructions: 5 L Maximum Qty/Pack: 852

Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity

Packing Instructions: 1 L Maximum Qty/Pack: Y841

Shipping Name: CORROSIVE LIQUID, N.O.S. *(CONTAINS 4-

FLUOROPHENYL ISOTHIOCYANATE)

Maritime Transport IMDG:

IMDG Class: 8 IMDG Subrisk: None

UN Number: 1760 Packing Group: III

EMS Number: F-A , S-B Special provisions: 223 274

Limited Quantities: 5 L

Shipping Name: CORROSIVE LIQUID, N.O.S.(contains 4-fluorophenyl isothiocyanate)

Section 15 - REGULATORY INFORMATION

4-fluorophenyl isothiocyanate (CAS: 1544-68-9) 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*.

* (limited evidence).

Denmark Advisory list for selfclassification of dangerous substances

Substance CAS Suggested codes 4- fluorophenyl isothiocyanate 1544- 68- 9 Xn; R22 R43 N; R50/53

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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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