

ALFAAL10891

## 3-Chloro-4-fluorophenyl isocyanate

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: 3-氯-4-氟苯异氰酸酯, 98%  
 Product Description: 3-Chloro-4-fluorophenyl isocyanate

Cat No. : L10891  
 CAS No 50529-33-4  
 Molecular Formula C7 H3 Cl F N O

Supplier Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
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E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

Physical State  
 Liquid

Appearance  
 Clear

Odor  
 No information available

#### Emergency Overview

Combustible liquid. Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

#### Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

#### Label Elements

**Signal Word****Warning****Hazard Statements**

H227 - Combustible liquid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed 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  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep 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  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P330 - Rinse mouth  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

**Other Hazards**

Lachrymator (substance which increases the flow of tears)  
This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
3-Chloro-4-fluorophenyl isocyanate	50529-33-4	98

**SECTION 4. FIRST AID MEASURES**

# SAFETY DATA SHEET

## 3-Chloro-4-fluorophenyl isocyanate

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

**Inhalation**

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

**Ingestion**

Clean mouth with water. Get medical attention.

**Most important symptoms and effects**

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

### SECTION 5. FIRE-FIGHTING MEASURES

**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Flammable. Combustible material. Containers may explode when heated.

**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.

### SECTION 6. ACCIDENTAL RELEASE MEASURES

**Personal Precautions**

Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

### SECTION 7. HANDLING AND STORAGE

**Handling**

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Keep away from open flames, hot surfaces and sources of ignition.

## 3-Chloro-4-fluorophenyl isocyanate

**Storage**

Keep container tightly closed. Keep refrigerated. Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

## 3-Chloro-4-fluorophenyl isocyanate

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When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Appearance	Clear	
Physical State	Liquid	
Odor	No information available	
Odor Threshold	No data available	
pH	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	44 °C / 111.2 °F	@ 17 mmHg
Flash Point	87 °C / 188.6 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	1.377	
Bulk Density	Not applicable	Liquid
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C7 H3 Cl F N O	
Molecular Weight	171.56	

**SECTION 10. STABILITY AND REACTIVITY**

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.
Materials to avoid	Strong oxidizing agents.
Hazardous Decomposition Products	Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). Hydrogen cyanide (hydrocyanic acid).

**SECTION 11. TOXICOLOGICAL INFORMATION**

## Product Information

# SAFETY DATA SHEET

## 3-Chloro-4-fluorophenyl isocyanate

(a) acute toxicity;	
(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects, both acute and delayed	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

### SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
Persistence and Degradability Persistence	No information available Persistence is unlikely, based on information available.
Bioaccumulative Potential	Bioaccumulation is unlikely
Mobility in soil	The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.
Endocrine Disruptor Information Persistent Organic Pollutant Ozone Depletion Potential	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance

### SECTION 13. DISPOSAL CONSIDERATIONS

## 3-Chloro-4-fluorophenyl isocyanate

**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

**Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport**

**UN-No** UN2206  
**Proper Shipping Name** ISOCYANATES, TOXIC, N.O.S.  
**Technical Shipping Name** 3-Chloro-4-fluorophenyl isocyanate  
**Hazard Class** 6.1  
**Packing Group** II

**IMDG/IMO**

**UN-No** UN2206  
**Proper Shipping Name** ISOCYANATES, TOXIC, N.O.S.  
**Technical Shipping Name** 3-Chloro-4-fluorophenyl isocyanate  
**Hazard Class** 6.1  
**Packing Group** II

**IATA**

**UN-No** UN2206  
**Proper Shipping Name** ISOCYANATE SOLUTION, TOXIC, N.O.S.  
**Technical Shipping Name** 3-Chloro-4-fluorophenyl isocyanate  
**Hazard Class** 6.1  
**Packing Group** II

**Special Precautions for User** No special precautions required

**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3-Chloro-4-fluorophenyl isocyanate	-	-	X	-	-	-	-	-	-	-	-	-

**National Regulations****SECTION 16. OTHER INFORMATION**

**3-Chloro-4-fluorophenyl isocyanate**

**Prepared By**  
**Revision Date**  
**Revision Summary**

Health, Safety and Environmental Department  
27-Apr-2024  
New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**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 Safety Data Sheet**