

SAFETY DATA SHEET

Version 6.6
Revision Date 08.03.2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 4-Fluorophenyl isocyanate

Product Number : F14335
Brand : Aldrich
CAS-No. : 1195-45-5

1.2 Other means of identification

No data available

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

1.4 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Pte Ltd
(Co. Registration No. 199403788W)
2 Science Park Drive
#05-01/12 Ascent Building
SINGAPORE 118222
SINGAPORE

Telephone : +65 6890 6633
Fax : +65 6890 6639
E-mail address : TechnicalService@merckgroup.com

1.5 Emergency telephone

Emergency Phone # : +65 3158 1349 (CHEMTREC intl.) 800 101
2201 (CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Serious eye damage/eye irritation (Category 2A), H319
Respiratory sensitization (Category 1), H334
Skin sensitization (Category 1), H317

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H226

Flammable liquid and vapor.

H302 + H312 + H332

Harmful if swallowed, in contact with skin or if inhaled.

H317

May cause an allergic skin reaction.

H319

Causes serious eye irritation.

H334

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary Statements

Prevention

P210

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P261

Avoid breathing mist or vapors.

P264

Wash skin thoroughly after handling.

P280

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

P284

Wear respiratory protection.

Response

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.

P304 + P340 + P312

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P342 + P311

If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

2.3 Other hazards

Lachrymator.

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Formula : C₇H₄FNO

Molecular weight : 137.11 g/mol

CAS-No. : 1195-45-5

EC-No. : 214-799-0

Hazardous ingredients

Component	Classification	Concentration
4-Fluorophenyl isocyanate		
	Flam. Liq. 3; Acute Tox. 4;	<= 100 %

	Eye Dam./Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; H226, H302, H332, H312, H319, H334, H317	
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For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 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.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NOx)

Hydrogen fluoride

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

5.3 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.

5.4 Further information

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

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability Recommended storage temperature

2 - 8 °C

Moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.3 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection**8.1 Control parameters****Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

8.2 Exposure controls**Appropriate engineering controls**

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

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

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols 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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties**

- | | |
|--|------------------------|
| a) Physical state | clear, liquid |
| b) Color | colorless |
| c) Odor | No data available |
| d) Melting point/freezing point | No data available |
| e) Initial boiling point and boiling range | 55 °C at 10 hPa - lit. |

f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	53 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient: n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	1.206 g/cm ³ at 25 °C - lit.
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat.

Heating.

10.5 Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - Expert judgment - 500.1 mg/kg

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 11.1 mg/l - vapor

Acute toxicity estimate Dermal - Expert judgment - 1,100.1 mg/kg

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Repeated exposure may cause asthma., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1993

IMDG: 1993

IATA-DGR: 1993

14.2 UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, N.O.S. (4-Fluorophenyl isocyanate) (4-Fluorophenyl isocyanate)

IMDG: FLAMMABLE LIQUID, N.O.S. (4-Fluorophenyl isocyanate) (4-Fluorophenyl isocyanate)

IATA-DGR: Flammable liquid, n.o.s. (4-Fluorophenyl isocyanate) (4-Fluorophenyl isocyanate)

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

None

14.7 Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

Other regulations

Hazchem Code : •3Y

SECTION 15: Regulatory information

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

No data available

SECTION 16: Other information

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Full text of H-Statements referred to under sections 2 and 3.

H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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