

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: **2-Fluorophenyl isocyanate**
Cat No. : **SB01843DA; SB01843ZZ**
Synonyms: o-Fluorophenyl isocyanate.
CAS No: 16744-98-2
Molecular Formula: C7 H4 F N O

1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use: Laboratory chemicals.
Uses advised against: No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
Thermo Fisher Scientific (Heysham),
Shore Road,
Port of Heysham Industrial Park,
Heysham, Lancashire, LA3 2XY
United Kingdom

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticaaan 3a
2440 Geel, Belgium

E-mail address: begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

Flammable liquids

Category 3 (H226)

Health hazards

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Acute oral toxicity
Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Respiratory Sensitization
Specific target organ toxicity - (single exposure)

Category 3 (H301)
Category 3 (H311)
Category 3 (H331)
Category 2 (H315)
Category 2 (H319)
Category 1 (H334)
Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H226 - Flammable liquid and vapor
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
H315 - Causes skin irritation
H335 - May cause respiratory irritation
H319 - Causes serious eye irritation
H301 + H311 + H331 - Toxic if swallowed, in contact with skin or if inhaled

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P342 + P311 - If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. 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

3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - Regulation (EC) No 1272/2008 |
|-----------|--------|-------|----------|---|
|-----------|--------|-------|----------|---|

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| | | | | |
|---------------------------|------------|-------------------|----|--|
| 2-Fluorophenyl isocyanate | 16744-98-2 | EEC No. 240-804-0 | 97 | STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Resp. Sens. 1 (H334) Acute Tox. 3 (H301) Acute Tox. 3 (H311) Acute Tox. 3 (H331) |
|---------------------------|------------|-------------------|----|--|

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

| | |
|---|--|
| Eye Contact | Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. |
| Skin Contact | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required. |
| Ingestion | Call a physician immediately. Clean mouth with water. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required. |
| 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. |

4.2. Most important symptoms and effects, both acute and delayed

Difficulty in breathing. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

4.3. Indication of any immediate medical attention and special treatment needed

| | |
|---------------------------|------------------------|
| Notes to Physician | Treat symptomatically. |
|---------------------------|------------------------|

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Do not use a solid water stream as it may scatter and spread fire. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

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Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic acid), Gaseous hydrogen fluoride (HF).

5.3. Advice 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

6.1. Personal precautions, protective equipment and emergency procedures

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

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Prevent product from entering drains. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not flush into surface water or sanitary sewer system.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Handle product only in closed system or provide appropriate exhaust ventilation. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharges.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 3
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

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SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

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 recommendations | - | EN 374 | (minimum requirement) |
| Neoprene | | | | |
| Natural rubber | | | | |
| PVC | | | | |

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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.

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

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| | |
|--|---|
| 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 When RPE is used a face piece Fit Test should be conducted |
| Environmental exposure controls | No information available. |

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

| | | |
|--|-------------------------------|--|
| Physical State | Liquid | |
| Appearance | Light brown | |
| Odor | Strong | |
| Odor Threshold | No data available | |
| Melting Point/Range | No data available | |
| Softening Point | No data available | |
| Boiling Point/Range | 56 - 58 °C / 132.8 - 136.4 °F | |
| Flammability (liquid) | Flammable | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Flash Point | 50 °C / 122 °F | Method - No information available |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | No data available | |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | No information available | |
| Vapor Pressure | No information available | |
| Density / Specific Gravity | 1.222 | |
| Bulk Density | Not applicable | Liquid |
| Vapor Density | 4.73 (Air = 1.0) | (Air = 1.0) |
| Particle characteristics | (liquid) Not applicable | |

9.2. Other information

| | |
|-----------------------------|--|
| Molecular Formula | C7 H4 F N O |
| Molecular Weight | 137.11 |
| Explosive Properties | explosive air/vapour mixtures possible |

SECTION 10: STABILITY AND REACTIVITY

| | |
|-------------------------|--|
| 10.1. Reactivity | None known, based on information available |
|-------------------------|--|

| | |
|---------------------------------|---|
| 10.2. Chemical stability | Stable under normal conditions. Moisture sensitive. |
|---------------------------------|---|

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10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions No information available.

10.4. Conditions to avoid

Excess heat. Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials

Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines.

10.6. Hazardous decomposition products

Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

| | |
|--|---|
| (a) acute toxicity; | |
| Oral | Category 3 |
| Dermal | Category 3 |
| Inhalation | Category 3 |
| (b) skin corrosion/irritation; | Category 2 |
| (c) serious eye damage/irritation; | Category 2 |
| (d) respiratory or skin sensitization; | |
| Respiratory | Category 1 |
| Skin | No data available |
| | No information 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. |

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(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. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

12.2. Persistence and degradability **Persistence**

No information available
Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

12.4. 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.

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors.

12.7. Other adverse effects **Persistent Organic Pollutant** **Ozone Depletion Potential**

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

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. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and

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empty container away from heat and sources of ignition.

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN3080
14.2. UN proper shipping name Isocyanate solution, toxic, flammable, n.o.s.
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

ADR

14.1. UN number UN3080
14.2. UN proper shipping name Isocyanate solution, toxic, flammable, n.o.s.
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

IATA

14.1. UN number UN3080
14.2. UN proper shipping name ISOCYANATE SOLUTION, TOXIC, FLAMMABLE, N.O.S.*
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component | CAS No | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|---------------------------|------------|-----------|--------|-----|-------|------|------|------|------|
| 2-Fluorophenyl isocyanate | 16744-98-2 | 240-804-0 | - | - | - | X | - | - | - |

| Component | CAS No | TSCA | TSCA Inventory | DSL | NDSL | AICS | NZIoC | PICCS |
|-----------|--------|------|----------------|-----|------|------|-------|-------|
|-----------|--------|------|----------------|-----|------|------|-------|-------|

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| | | | | | | | | |
|---------------------------|------------|---|-----------------------------------|---|---|---|---|---|
| | | | notification - Active-Inactive | | | | | |
| 2-Fluorophenyl isocyanate | 16744-98-2 | - | - | - | - | - | - | - |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|---------------------------|------------|---|--|---|
| 2-Fluorophenyl isocyanate | 16744-98-2 | - | - | - |

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|---------------------------|------------|---|--|
| 2-Fluorophenyl isocyanate | 16744-98-2 | Not applicable | Not applicable |

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

Water endangering class = 3 (self classification)

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H301 - Toxic if swallowed

H311 - Toxic in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H331 - Toxic if inhaled

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

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H335 - May cause respiratory irritation

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/NDL - 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

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

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

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

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

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

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

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

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

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.

Revision Date

01-Sep-2023

Revision Summary

SDS sections updated, 1, 9, 2, 11, 12, 15, 16.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.
COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No
1907/2006**

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