

SAFETY DATA SHEET

Revision Date 23-Jul-2021

Revision Number 3

1. Identification

Product Name 3-Fluorophenyl isothiocyanate

Cat No. : B25001

CAS No 404-72-8
Synonyms 1-Fluoropyridinium pyridine heptafluorodiborate; M-Fluorophenyl isothiocyanate

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

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
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid
Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
Call a POISON CENTER or doctor/physician if you feel unwell
If skin irritation occurs: Get medical advice/attention
Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Benzene, 1-fluoro-3-isothiocyanato-	404-72-8	99.0

4. First-aid measures

General Advice	If symptoms persist, call a physician.
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 plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Most important symptoms and effects	Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	84 °C / 183.2 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Combustible material. Containers may explode when heated.

Hazardous Combustion Products

None known.

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.

NFPA

Health
2

Flammability
2

Instability
0

Physical hazards
N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
Environmental Precautions	Should not be released into the environment. See Section 12 for additional Ecological Information.
Methods for Containment and Clean Up	Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not
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get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition.

Storage

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

8. Exposure controls / personal protection

Exposure Guidelines

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

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment**Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Yellow
Odor	No information available
Odor Threshold	No information available
pH	
Melting Point/Range	No data available
Boiling Point/Range	227 °C / 440.6 °F
Flash Point	84 °C / 183.2 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	5.28
Specific Gravity	1.2700
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C7H4FNS
Molecular Weight	153.18

10. Stability and reactivity

Reactive Hazard

None known, based on information available

Stability	Stable under normal conditions.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	None under normal use conditions
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Benzene, 1-fluoro-3-isothiocyanato-	404-72-8	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability No information available

Bioaccumulation/ Accumulation No information available.

Mobility No information available.

13. Disposal considerations

Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk.

UN-No

NA1993

Proper Shipping Name

Combustible liquid, n.o.s.

Packing Group

III

TDG

Not regulated

IATA

Not regulated

IMDG/IMO

Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
Benzene, 1-fluoro-3-isothiocyanato-	404-72-8	X	INACTIVE	-

Legend:

TSCA - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Benzene, 1-fluoro-3-isothiocyanato-	404-72-8	-	X	206-967-7	-	-		-	-	-

U.S. Federal Regulations

SARA 313

Not applicable

SARA 311/312 Hazard Categories

See section 2 for more information

CWA (Clean Water Act)

Not applicable

Clean Air Act

Not applicable

OSHA - Occupational Safety and Health Administration

Not applicable

CERCLA

Not applicable

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

16. Other information

Prepared By Health, Safety and Environmental Department
Email: tech@alfa.com
www.alfa.com

Revision Date 23-Jul-2021

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Revision Summary SDS authoring systems update, replaces ChemGes SDS No. 404-72-8/2.

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 SDS