

## 1 Identification

### Product identifier

**Product name:** 2,4,6-Trifluorophenyl isocyanate

**Stock number:** L19349

**CAS Number:**

50528-80-8

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

**Identified use:** SU24 Scientific research and development

### Details of the supplier of the safety data sheet

#### Manufacturer/Supplier:

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

**Information Department:** Health, Safety and Environmental Department

#### 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 of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS02 Flame

Flam. Liq. 3 H226 Flammable liquid and vapour.



GHS06 Skull and crossbones

Acute Tox. 2 H330 Fatal if inhaled.



GHS08 Health hazard

Resp. Sens. 1 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Muta. 1A H340 May cause genetic defects.

Carc. 1A H350 May cause cancer.

STOT RE 1 H372 Causes damage to organs through prolonged or repeated exposure.

**Hazards not otherwise classified** Lachrymator

### Label elements

**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

### Hazard pictograms



GHS02 GHS06 GHS08

### Signal word

**Danger**

### Hazard statements

H226 Flammable liquid and vapour.

H330 Fatal if inhaled.

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

H340 May cause genetic defects.

H350 May cause cancer.

H372 Causes damage to organs through prolonged or repeated exposure.

### Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P320 Specific treatment is urgent (see on this label).

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

### WHMIS classification

B3 - Combustible liquid

D1A - Very toxic material causing immediate and serious toxic effects

D2A - Very toxic material causing other toxic effects



### Classification system

**HMIS ratings (scale 0-4)**

**(Hazardous Materials Identification System)**

HEALTH **3** Health (acute effects) = 3

FIRE **2** Flammability = 2

REACTIVITY **1** Physical Hazard = 1

### Other hazards

### Results of PBT and vPvB assessment

**PBT:** Not applicable.

**vPvB:** Not applicable.

Product name: **2,4,6-Trifluorophenyl isocyanate**

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**3 Composition/information on ingredients**

**Chemical characterization: Substances**  
**CAS# Description:**  
50528-80-8 2,4,6-Trifluorophenyl isocyanate

**4 First-aid measures**

**Description of first aid measures**  
**General information**  
Immediately remove any clothing soiled by the product.  
Remove breathing apparatus only after contaminated clothing has been completely removed.  
In case of irregular breathing or respiratory arrest provide artificial respiration.  
**After inhalation**  
Supply fresh air. If required, provide artificial respiration. Keep patient warm.  
Seek immediate medical advice.  
**After skin contact**  
Immediately wash with water and soap and rinse thoroughly.  
Seek immediate medical advice.  
**After eye contact** Rinse opened eye for several minutes under running water. Then consult a doctor.  
**After swallowing** Seek medical treatment.  
**Information for doctor**  
**Most important symptoms and effects, both acute and delayed** No further relevant information available.  
**Indication of any immediate medical attention and special treatment needed** No further relevant information available.

**5 Fire-fighting measures**

**Extinguishing media**  
**Suitable extinguishing agents** CO2, sand, extinguishing powder. Do not use water.  
**Special hazards arising from the substance or mixture**  
If this product is involved in a fire, the following can be released:  
Carbon monoxide and carbon dioxide  
Nitrogen oxides (NOx)  
Hydrogen cyanide (HCN)  
Hydrogen fluoride (HF)  
**Advice for firefighters**  
**Protective equipment:**  
Wear self-contained respirator.  
Wear fully protective impervious suit.

**6 Accidental release measures**

**Personal precautions, protective equipment and emergency procedures**  
Wear protective equipment. Keep unprotected persons away.  
Ensure adequate ventilation  
Keep away from ignition sources  
**Environmental precautions:** Do not allow material to be released to the environment without proper governmental permits.  
**Methods and material for containment and cleaning up:**  
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).  
Dispose of contaminated material as waste according to section 13.  
Ensure adequate ventilation.  
**Prevention of secondary hazards:** Keep away from ignition sources.  
**Reference to other sections**  
See Section 7 for information on safe handling  
See Section 8 for information on personal protection equipment.  
See Section 13 for disposal information.

**7 Handling and storage**

**Handling**  
**Precautions for safe handling**  
Handle under dry protective gas.  
Keep container tightly sealed.  
Ensure good ventilation at the workplace.  
Open and handle container with care.  
**Information about protection against explosions and fires:**  
Keep ignition sources away.  
Protect against electrostatic charges.  
Fumes can combine with air to form an explosive mixture.  
**Conditions for safe storage, including any incompatibilities**  
**Storage**  
**Requirements to be met by storerooms and receptacles:** Refrigerate  
**Information about storage in one common storage facility:**  
Store away from oxidizing agents.  
Protect from heat.  
Store away from water/moisture.  
**Further information about storage conditions:**  
Store under dry inert gas.  
This product is moisture sensitive.  
Keep container tightly sealed.  
Protect from humidity and water.  
Refrigerate  
**Specific end use(s)** No further relevant information available.

**8 Exposure controls/personal protection**

**Additional information about design of technical systems:**  
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.  
**Control parameters**  
**Components with limit values that require monitoring at the workplace:** Not required.  
**Additional information:** No data

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**Exposure controls**

**Personal protective equipment**

**General protective and hygienic measures**

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Maintain an ergonomically appropriate working environment.

**Breathing equipment:** Use self-contained respiratory protective device in emergency situations.

**Protection of hands:**

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

**Penetration time of glove material (in minutes)** Not determined

**Eye protection:** Safety glasses

**Body protection:** Protective work clothing.

**9 Physical and chemical properties**

**Information on basic physical and chemical properties**

**General Information**

**Appearance:**

**Form:** Liquid  
**Color:** Colorless  
**Odor:** Pungent  
**Odor threshold:** Not determined.

**pH-value:** Not determined.

**Change in condition**

**Melting point/Melting range:** Not determined  
**Boiling point/Boiling range:** Not determined  
**Sublimation temperature / start:** Not determined

**Flash point:** < 60 °C (< 140 °F)  
**Flammability (solid, gaseous)** Not determined.  
**Ignition temperature:** Not determined  
**Decomposition temperature:** Not determined  
**Auto igniting:** Not determined.

**Danger of explosion:** Not determined.

**Explosion limits:**

**Lower:** Not determined  
**Upper:** Not determined  
**Vapor pressure:** Not determined  
**Density:** Not determined  
**Relative density** Not determined.  
**Vapor density** Not determined.  
**Evaporation rate** Not determined.

**Solubility in / Miscibility with**

**Water:** Hydrolyzes  
**Partition coefficient (n-octanol/water):** Not determined.

**Viscosity:**

**dynamic:** Not determined.  
**kinematic:** Not determined.

**Other information** No further relevant information available.

**10 Stability and reactivity**

**Reactivity** No information known.

**Chemical stability** Stable under recommended storage conditions.

**Thermal decomposition / conditions to be avoided:** Decomposition will not occur if used and stored according to specifications.

**Possibility of hazardous reactions** No dangerous reactions known

**Conditions to avoid** No further relevant information available.

**Incompatible materials:**

Oxidizing agents

Alcohols

Amines

Water/moisture

Heat

**Hazardous decomposition products:**

Carbon monoxide and carbon dioxide

Nitrogen oxides

Hydrogen fluoride

Hydrogen cyanide

**11 Toxicological information**

**Information on toxicological effects**

**Acute toxicity:** Fatal if inhaled.

**LD/LC50 values that are relevant for classification:** No data

**Skin irritation or corrosion:** Irritant to skin and mucous membranes.

**Eye irritation or corrosion:**

This product is a lachrymator.

Lachrymator. Produces tears and temporary eye irritation.

**Sensitization:** May cause allergy or asthma symptoms or breathing difficulties if inhaled.

**Germ cell mutagenicity:** May cause genetic defects.

**Carcinogenicity:**

May cause cancer.

No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

**Reproductive toxicity:** No effects known.

**Specific target organ system toxicity - repeated exposure:**

Causes damage to organs through prolonged or repeated exposure.

Specific target organ is not known.

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USA

Product name: **2,4,6-Trifluorophenyl isocyanate**

**Specific target organ system toxicity - single exposure:** No effects known.  
**Aspiration hazard:** No effects known.  
**Subacute to chronic toxicity:** No effects known.  
**Subacute to chronic toxicity:**  
Isocyanates are extremely irritating to the skin, eyes and mucous membranes. Exposure may be fatal. Symptoms include burning sensation, coughing, wheezing, laryngitis, headache, nausea and vomiting.  
**Additional toxicological information:** To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.





12 Ecological information

**Toxicity**  
**Aquatic toxicity:** No further relevant information available.  
**Persistence and degradability** No further relevant information available.  
**Bioaccumulative potential** No further relevant information available.  
**Mobility in soil** No further relevant information available.  
**Additional ecological information:**  
**General notes:**  
Do not allow material to be released to the environment without proper governmental permits.  
Do not allow product to reach ground water, water course or sewage system, even in small quantities.  
Danger to drinking water if even extremely small quantities leak into the ground.  
Avoid transfer into the environment.  
**Results of PBT and vPvB assessment**  
**PBT:** Not applicable.  
**vPvB:** Not applicable.  
**Other adverse effects** No further relevant information available.




13 Disposal considerations

**Waste treatment methods**  
**Recommendation** Consult state, local or national regulations to ensure proper disposal.  
**Uncleaned packagings:**  
**Recommendation:** Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN3080
UN proper shipping name DOT IMDG, IATA	Isocyanates, toxic, flammable, n.o.s. (2,4,6-Trifluorophenyl isocyanate) ISOCYANATES, TOXIC, FLAMMABLE, N.O.S. (2,4,6-Trifluorophenyl isocyanate)
Transport hazard class(es) DOT	 
Class Label Class Label IMDG, IATA	6.1 Toxic substances. 6.1+3 6.1 (TF1) Toxic substances 6.1+3
 	
Class Label	6.1 Toxic substances. 6.1+3
Packing group DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user EMS Number:	Warning: Toxic substances F-E,S-D
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3080, Isocyanates, toxic, flammable, n.o.s. (2,4,6-Trifluorophenyl isocyanate), 6.1 (3), II

15 Regulatory information

**Safety, health and environmental regulations/legislation specific for the substance or mixture**  
**GHS label elements** The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)  
**Hazard pictograms**  
  
GHS02 GHS06 GHS08  
**Signal word** Danger  
**Hazard statements**  
H226 Flammable liquid and vapour.  
H330 Fatal if inhaled.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H340 May cause genetic defects.  
H350 May cause cancer.  
H372 Causes damage to organs through prolonged or repeated exposure.

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Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.  
P320 Specific treatment is urgent (see on this label).  
P405 Store locked up.  
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use:

For use only by technically qualified individuals.

Workers are not allowed to be exposed to this hazardous material. Exceptions can be made by the authorities in certain cases.

Other regulations, limitations and prohibitive regulations

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation / last revision 11/24/2015 / -

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)