

## 1 Identification

### Product identifier

**Product name:** 3-(Trifluoromethyl)phenyl isocyanate

**Stock number:** L09448

**CAS Number:**  
329-01-1

**EC number:**  
206-341-3

**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. 3 H301 Toxic if swallowed.

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.



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

**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.

H301 Toxic if swallowed.

H330 Fatal if inhaled.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

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

H335 May cause respiratory irritation.

### Precautionary statements

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

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...

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

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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



**Product name: 3-(Trifluoromethyl)phenyl isocyanate**

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**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.

**3 Composition/information on ingredients**

**Chemical characterization: Substances**  
**CAS# Description:**  
329-01-1 3-(Trifluoromethyl)phenyl isocyanate  
**Identification number(s):**  
**EC number:** 206-341-3

**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  
Hydrogen fluoride (HF)  
Nitrogen oxides (NOx)  
Hydrogen cyanide (HCN)  
**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  
**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:** No special measures required.  
**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.  
Prevent formation of aerosols.  
**Information about protection against explosions and fires:** Keep ignition sources away.  
**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

(Contd. on page 3)  
USA

<b>Product name: 3-(Trifluoromethyl)phenyl isocyanate</b>	
<b>Specific end use(s)</b> No further relevant information available.	
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<b>8 Exposure controls/personal protection</b>	
<b>Additional information about design of technical systems:</b> Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.	
<b>Control parameters</b>	
<b>Components with limit values that require monitoring at the workplace:</b> Not required.	
<b>Additional information:</b> No data	
<b>Exposure controls</b>	
<b>Personal protective equipment</b>	
<b>General protective and hygienic measures</b> 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. Avoid contact with the eyes and skin. Maintain an ergonomically appropriate working environment.	
<b>Breathing equipment:</b> Use self-contained respiratory protective device in emergency situations.	
<b>Protection of hands:</b> 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.	
<b>Penetration time of glove material (in minutes)</b> Not determined	
<b>Eye protection:</b> Safety glasses	
<b>Body protection:</b> Protective work clothing.	
<b>9 Physical and chemical properties</b>	
<b>Information on basic physical and chemical properties</b>	
<b>General Information</b>	
<b>Appearance:</b>	
<b>Form:</b>	Liquid
<b>Color:</b>	Colorless
<b>Odor:</b>	Pungent
<b>Odor threshold:</b>	Not determined.
<b>pH-value:</b>	Not determined.
<b>Change in condition</b>	
<b>Melting point/Melting range:</b>	Not determined
<b>Boiling point/Boiling range:</b>	53-54 °C (127-129 °F) (11 mmHg)
<b>Sublimation temperature / start:</b>	Not determined
<b>Flash point:</b>	58 °C (136 °F)
<b>Flammability (solid, gaseous)</b>	Not determined.
<b>Ignition temperature:</b>	Not determined
<b>Decomposition temperature:</b>	Not determined
<b>Auto igniting:</b>	Not determined.
<b>Danger of explosion:</b>	Product does not present an explosion hazard.
<b>Explosion limits:</b>	
<b>Lower:</b>	Not determined
<b>Upper:</b>	Not determined
<b>Vapor pressure:</b>	Not determined
<b>Density at 20 °C (68 °F):</b>	1.336 g/cm³ (11.149 lbs/gal)
<b>Relative density</b>	Not determined.
<b>Vapor density</b>	Not determined.
<b>Evaporation rate</b>	Not determined.
<b>Solubility in / Miscibility with</b>	
<b>Water:</b>	Hydrolyzes
<b>Partition coefficient (n-octanol/water):</b>	Not determined.
<b>Viscosity:</b>	
<b>dynamic:</b>	Not determined.
<b>kinematic:</b>	Not determined.
<b>Other information</b>	No further relevant information available.
<b>10 Stability and reactivity</b>	
<b>Reactivity</b> No information known.	
<b>Chemical stability</b> Stable under recommended storage conditions.	
<b>Thermal decomposition / conditions to be avoided:</b> Decomposition will not occur if used and stored according to specifications.	
<b>Possibility of hazardous reactions</b> No dangerous reactions known	
<b>Conditions to avoid</b> No further relevant information available.	
<b>Incompatible materials:</b>	
Alcohols	
Amines	
Oxidizing agents	
Heat	
Water/moisture	
<b>Hazardous decomposition products:</b>	
Carbon monoxide and carbon dioxide	
Hydrogen fluoride	
Nitrogen oxides	
Hydrogen cyanide	
<b>11 Toxicological information</b>	
<b>Information on toxicological effects</b>	
<b>Acute toxicity:</b>	
Harmful if swallowed.	
Fatal if inhaled.	
<b>LD/LC50 values that are relevant for classification:</b> No data	
<b>Skin irritation or corrosion:</b> Causes skin irritation.	
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Product name: **3-(Trifluoromethyl)phenyl isocyanate**

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**Eye irritation or corrosion:**  
Causes serious eye irritation.  
This product is a lachrymator.  
**Sensitization:** May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
**Germ cell mutagenicity:** No effects known.  
**Carcinogenicity:** 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:** No effects known.  
**Specific target organ system toxicity - single exposure:** May cause respiratory irritation.  
**Aspiration hazard:** No effects known.  
**Subacute to chronic toxicity:**  
The Registry of Toxic Effects of Chemical Substances (RTECS) reports the following effects in laboratory animals:  
Behavioral - somnolence (general depressed activity).  
Behavioral - convulsions or effect on seizure threshold.  
Lungs, Thorax, or Respiration - cyanosis.  
Lungs, Thorax, or Respiration - other changes.  
Gastrointestinal - other changes.  
Brain and Coverings - other degenerative changes.  
Cardiac - other changes.  
Liver - other changes.  
Tumorigenic - active as anti-cancer agent.  
Sense Organs and Special Senses (Olfaction) - deviated nasal septum.  
**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 undiluted product or large quantities to reach ground water, water course or sewage system.  
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	UN2285
UN proper shipping name DOT IMDG, IATA	Isocyanatobenzotrifluorides ISOCYANATOBENZOTRIFLUORIDES
Transport hazard class(es) DOT 	6.1 Toxic substances. 6.1+3 6.1 (TF1) Toxic substances 6.1+3
Class Label Class Label IMDG, IATA 	6.1 Toxic substances. 6.1+3
Packing group DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Toxic substances
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":	UN2285, Isocyanatobenzotrifluorides, 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)

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USA

**Product name: 3-(Trifluoromethyl)phenyl isocyanate**

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**Hazard pictograms**



GHS02 GHS06 GHS08

**Signal word** *Danger*

**Hazard statements**

H226 *Flammable liquid and vapour.*  
H301 *Toxic if swallowed.*  
H330 *Fatal if inhaled.*  
H315 *Causes skin irritation.*  
H319 *Causes serious eye irritation.*  
H334 *May cause allergy or asthma symptoms or breathing difficulties if inhaled.*  
H335 *May cause respiratory irritation.*

**Precautionary statements**

P210 *Keep away from heat/sparks/open flames/hot surfaces. No smoking.*  
P301+P310 *IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...*  
P303+P361+P353 *If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.*  
P305+P351+P338 *IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.*  
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**

All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.  
All components of this product are listed on the Canadian Non-Domestic Substances List (NDSL).

**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.

**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** 11/23/2015 / -

**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

EINECS: European Inventory of Existing Commercial Chemical Substances

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)