

1 Identification

Product identifier

Product name: 4-(Trifluoromethyl)phenyl isocyanate

Stock number: L12576

CAS Number:

1548-13-6

EC number:

218-925-5

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)



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.



GHS07

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

H227 Combustible liquid.

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



GHS06 GHS08

Signal word

Danger

Hazard statements

H227 Combustible liquid.

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.

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

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



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.

Product name: 4-(Trifluoromethyl)phenyl isocyanate	
vPvB: Not applicable.	(Contd. of page 1)
3 Composition/information on ingredients Chemical characterization: Substances CAS# Description: 1548-13-6 4-(Trifluoromethyl)phenyl isocyanate Identification number(s): EC number: 218-925-5	
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 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. 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 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	

Product name: 4-(Trifluoromethyl)phenyl isocyanate

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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.

Avoid contact with the eyes and skin.

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: 91-94 °C (196-201 °F) (35 mmHg)

Sublimation temperature / start: Not determined

Flash point: 70 °C (158 °F)

Flammability (solid, gaseous) Not determined.

Ignition temperature: Not determined

Decomposition temperature: Not determined

Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.

Explosion limits:

Lower: Not determined

Upper: Not determined

Vapor pressure: Not determined

Density at 20 °C (68 °F): 1.31 g/cm³ (10.932 lbs/gal)

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 Isocyanates may react exothermically with NH, OH or SH groups

Conditions to avoid No further relevant information available.

Incompatible materials:

Alcohols

Amines

Oxidizing agents

Heat

Water/moisture

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: Causes skin irritation.

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: No effects known.

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USA

Product name: 4-(Trifluoromethyl)phenyl isocyanate	
<div><div>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.</div><div>(Contd. of page 3)</div></div>	
12 Ecological information <div><div>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.</div></div>	
13 Disposal considerations <div><div>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.</div></div>	
14 Transport information	
UN-Number DOT, IMDG, IATA	UN2285
UN proper shipping name DOT IMDG, IATA	Isocyanatobenzotrifluorides ISOCYANATOBENZOTRIFLUORIDES
Transport hazard class(es) DOT	<div><div></div><div>Class Label Class Label IMDG, IATA</div><div>6.1 Toxic substances. 6.1+3 6.1 (TF1) Toxic substances 6.1+3</div></div>
<div><div></div><div>Class Label</div><div>6.1 Toxic substances. 6.1+3</div></div>	
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 <div><div>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 <div><div></div><div>GHS06 GHS08</div></div><div>Signal word Danger Hazard statements H227 Combustible liquid. 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. P260 Do not breathe dust/fume/gas/mist/vapours/spray. 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.</div></div></div>	
<div>(Contd. on page 5) USA</div>	

Product name: 4-(Trifluoromethyl)phenyl isocyanate

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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.
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)

USA