

1 Identification

Product identifier

Product name: **3,5-Bis(trifluoromethyl)phenyl isocyanate**

Stock number: L09582

CAS Number:
 16588-74-2

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. 3 H331 Toxic if inhaled.



GHS08 Health hazard

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



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

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.

H302 Harmful if swallowed.

H331 Toxic 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

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

P280 Wear protective gloves / protective clothing.

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

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER/doctor/...

WHMIS classification

B3 - Combustible liquid

D1B - 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 2 Health (acute effects) = 2

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: **3,5-Bis(trifluoromethyl)phenyl isocyanate**

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3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

16588-74-2 3,5-Bis(trifluoromethyl)phenyl isocyanate

4 First-aid measures

Description of first aid measures

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 (NO_x)

Possibly 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.

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

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.

Do not inhale gases / fumes / aerosols.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

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USA

Product name: **3,5-Bis(trifluoromethyl)phenyl isocyanate**

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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: 62 °C (144 °F) (2 mmHg)
Sublimation temperature / start: Not determined

Flash point: 67 °C (153 °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): 1.476 g/cm³ (12.317 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 No dangerous reactions known

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
Possibly Hydrogen cyanide (HCN)

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful if swallowed.

Toxic 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.

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.

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USA

Product name: 3,5-Bis(trifluoromethyl)phenyl isocyanate



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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	UN2206
UN proper shipping name DOT IMDG, IATA	Isocyanates, toxic, n.o.s. (3,5-Bis(trifluoromethyl)phenyl isocyanate) ISOCYANATES, TOXIC, N.O.S. (3,5-Bis(trifluoromethyl)phenyl isocyanate)
Transport hazard class(es) DOT	
	
Class Label Class Label IMDG, IATA	6.1 Toxic substances. 6.1 6.1 (T1) Toxic substances 6.1
	
Class Label	6.1 Toxic substances. 6.1
Packing group DOT, IMDG, IATA	III
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":	UN2206, Isocyanates, toxic, n.o.s. (3,5-Bis(trifluoromethyl)phenyl isocyanate), 6.1, III

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



GHS06 GHS08

Signal word Danger

Hazard statements

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P309 IF exposed or if you feel unwell:
P310 Immediately call a POISON CENTER/doctor/...

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.

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Product name: 3,5-Bis(trifluoromethyl)phenyl isocyanate

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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 11/24/2015 / -

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)