

## SAFETY DATA SHEET

Creation Date 23-Oct-2010

Revision Date 14-Feb-2020

Revision Number 2

### 1. Identification

**Product Name** 4-(Trifluoromethoxy)phenyl isocyanate

**Cat No. :** B20033

**CAS-No** 35037-73-1

**Synonyms** 1-Isocyanato-4-(trifluoromethoxy)benzene

**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 3
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 1 C
Serious Eye Damage/Eye Irritation	Category 1
Respiratory Sensitization	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

**Label Elements**

**Signal Word**

Danger

**Hazard Statements**

Combustible liquid  
Harmful if swallowed  
Toxic in contact with skin  
Causes severe skin burns and eye damage  
May cause respiratory irritation  
May cause an allergic skin reaction  
Fatal if inhaled  
May cause allergy or asthma symptoms or breathing difficulties 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  
Do not breathe dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area  
Wear respiratory protection  
In case of inadequate ventilation wear respiratory protection  
Contaminated work clothing should not be allowed out of the workplace  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
Keep cool

**Response**

Immediately call a POISON CENTER or doctor/physician

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

**Skin**

Wash contaminated clothing before reuse  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
If skin irritation or rash occurs: Get medical advice/attention

**Eyes**

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

**Ingestion**

Rinse mouth  
Do NOT induce vomiting

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**Storage**

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

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Harmful to aquatic life with long lasting effects

### 3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	>95

## 4. First-aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Remove to fresh air. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms and effects</b>	Causes burns by all exposure routes. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
<b>Notes to Physician</b>	Treat symptomatically

## 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray, carbon dioxide (CO <sub>2</sub> ), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	69 °C / 156.2 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

### Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Combustible material. Containers may explode when heated.

### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF).

### 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. Thermal decomposition can lead to release of irritating gases and vapors.

### NFPA

Health  
4Flammability  
2Instability  
0Physical hazards  
N/A**6. Accidental release measures**

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	Should not be released into the environment. Do not flush into surface water or sanitary sewer system.
<b>Methods for Containment and Clean Up</b>	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

**7. Handling and storage**

<b>Handling</b>	Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition.
<b>Storage</b>	Keep in a dry place. Keep container tightly closed. Keep away from heat, sparks and flame. Store under an inert atmosphere. Keep refrigerated. Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

**8. Exposure controls / personal protection**

<b>Exposure Guidelines</b>	This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.
<b>Engineering Measures</b>	Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.
<b>Personal Protective Equipment</b>	
<b>Eye/face Protection</b>	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.
<b>Skin and body protection</b>	Wear appropriate protective gloves and clothing to prevent skin exposure.
<b>Respiratory Protection</b>	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.
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.

**9. Physical and chemical properties**

<b>Physical State</b>	Liquid
<b>Appearance</b>	Clear
<b>Odor</b>	No information available
<b>Odor Threshold</b>	No information available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	No data available
<b>Boiling Point/Range</b>	78 °C / 172.4 °F @ 22 mmHg
<b>Flash Point</b>	69 °C / 156.2 °F
<b>Evaporation Rate</b>	No information available
<b>Flammability (solid,gas)</b>	Not applicable

**Flammability or explosive limits**

Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	7.0
Specific Gravity	1.340
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	C8 H4 F3 N O2
Molecular Weight	203.12
Refractive index	1.457-1.460

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Stable. Moisture sensitive.
<b>Conditions to Avoid</b>	Excess heat. Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Strong oxidizing agents, Alcohols, Amines, Water
<b>Hazardous Decomposition Products</b>	Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Hydrogen cyanide (hydrocyanic acid), Gaseous hydrogen fluoride (HF)
<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

**Acute Toxicity****Product Information****Component Information**

<b>Toxicologically Synergistic Products</b>	No information available
---	--------------------------

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

<b>Irritation</b>	No information available
<b>Sensitization</b>	May cause sensitization by skin contact
<b>Carcinogenicity</b>	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	Not listed	Not listed	Not listed	Not listed	Not listed

<b>Mutagenic Effects</b>	No information available
--------------------------	--------------------------

<b>Reproductive Effects</b>	No information available.
-----------------------------	---------------------------

<b>Developmental Effects</b>	No information available.
------------------------------	---------------------------

<b>Teratogenicity</b>	No information available.
-----------------------	---------------------------

<b>STOT - single exposure</b>	Respiratory system
<b>STOT - repeated exposure</b>	None known
<b>Aspiration hazard</b>	No information available
<b>Symptoms / effects, both acute and delayed</b>	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
<b>Endocrine Disruptor Information</b>	No information available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

<b>Persistence and Degradability</b>	Persistence is unlikely based on information available.
<b>Bioaccumulation/ Accumulation</b>	No information available.
<b>Mobility</b>	Will likely be mobile in the environment due to its volatility.

## 13. Disposal considerations

<b>Waste Disposal Methods</b>	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

<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Technical Name</b>	Benzene, 1-isocyanato-4-(trifluoromethoxy)-
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I

### TDG

<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I

### IATA

	FORBIDDEN FOR IATA TRANSPORT
<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.*
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8

### IMDG/IMO

<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I

## 15. Regulatory information

**United States of America Inventory**

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	X	ACTIVE	PMN

**Legend:**

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

X - Listed

'-' - Not Listed

PMN - Indicates a commenced PMN substance

TSCA 12(b) - Notices of Export Not applicable

**International Inventories**

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

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	-	X	252-328-0	-	-	-	-	-

**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

<b>Creation Date</b>	23-Oct-2010
<b>Revision Date</b>	14-Feb-2020
<b>Print Date</b>	14-Feb-2020
<b>Revision Summary</b>	SDS authoring systems update, replaces ChemGes SDS No. 35037-73-1.

**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**