4-Chlorobenzotrifluoride

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
SDS Reference Number: 1800704
Issue date: 12/17/2015 Revision date: 7/30/2026 Version: 1.1

SECTION 1 Identification

1.1. Product identifier

Product form	:	Substance
Substance name	:	4-Chlorobenzotrifluoride
CAS-No.	:	98-56-6
Product code	:	1800-7-04
Formula	:	C7H4ClF3

1.2. Other means of identification

Synonyms	:	1-Chloro-4-(trifluoromethyl)benzene; 4-Chloro-alpha,alpha,alpha-trifluorotoluene
Other means of identification	:	MFCD00000627
EC-No.	:	202-681-1

1.3. Recommended use of the chemical and restrictions on use

Use of the substance/mixture	:	Laboratory chemicals,Manufacture of substances,Scientific research and development

1.4. Supplier's details

SynQuest Laboratories, Inc.
P.O. Box 309
Alachua, FL, Alachua, 32615
United States of America
T (386) 462-0788 - F (386) 462-7097
info@synquestlabs.com - www.synquestlabs.com

1.5. Emergency phone number

Emergency number	:	(844) 523-4086 (3E Company - Account 10069)

SECTION 2 Hazard Identification

2.1. Classification of the substance or mixture

GHS US classification

Flammable liquids, Category 3	H226	Flammable liquid and vapor.
Skin corrosion/irritation, Category 2	H315	Causes skin irritation.
Serious eye damage/eye irritation, Category 2A	H319	Causes serious eye irritation.
Skin sensitization, Category 1	H317	May cause an allergic skin reaction.
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation.
Hazardous to the aquatic environment — Acute Hazard, Category 2	H401	Toxic to aquatic life.
Hazardous to the aquatic environment — Chronic Hazard, Category 2	H411	Toxic to aquatic life with long lasting effects.

Full text of H statements : see section 16

2.2. Label elements

GHS US labeling

Hazard pictograms (GHS US) :

Signal word (GHS US) : Warning

Hazard statements (GHS US)	:	H226 - Flammable liquid and vapor H315 - Causes skin irritation H317 - May cause an allergic skin reaction H319 - Causes serious eye irritation H335 - May cause respiratory irritation H411 - Toxic to aquatic life with long lasting effects
Precautionary statements (GHS US)	:	P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P233 - Keep container tightly closed. P240 - Ground/Bond container and receiving equipment. P241 - Use explosion-proof equipment. P242 - Use non-sparking tools. P243 - Take action to prevent static discharges. P261 - Avoid breathing dust, fume, gas, mist, vapours, spray. P264 - Wash hands, forearms and face thoroughly after handling. P271 - Use only outdoors or in a well-ventilated area. P272 - Contaminated work clothing must not be allowed out of the workplace. P273 - Avoid release to the environment. P280 - Wear protective gloves. P302+P352 - If on skin: Wash with plenty of soap and water P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing. P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing P312 - Call a POISON CENTER or doctor/physician if you feel unwell P321 - Specific treatment (see supplemental first aid instruction on this label). P333+P313 - If skin irritation or rash occurs: Get medical advice or attention. P337+P313 - If eye irritation persists: Get medical advice or attention. P362+P364 - Take off contaminated clothing and wash it before reuse. P370+P378 - In case of fire: Use appropriate media to extinguish. P391 - Collect spillage. P403+P233 - Store in a well-ventilated place. Keep container tightly closed. P403+P235 - Store in a well-ventilated place. Keep cool. P405 - Store locked up. P501 - Dispose of contents and/or container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulations.

2.3. Hazards associated with known or reasonably anticipated uses

No additional information available

2.4. Hazards not otherwise classified

No additional information available

2.5. Unknown acute toxicity

No additional information available

SECTION 3 Composition/information on ingredients

3.1. Substances

Substance type	:	Mono-constituent

Name	Product identifier	%	GHS US classification
4-Chlorobenzotrifluoride (Main constituent)	CAS-No.: 98-56-6	≤ 100	Flam. Liq. 3, H226 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 Skin Sens. 1, H317 STOT SE 3, H335 Aquatic Acute 2, H401 Aquatic Chronic 2, H411

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4 First aid measures

4.1. Description of necessary first-aid measures

First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get medical advice/attention.

First-aid measures after skin contact : Wash with plenty of soap and water. Get medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

4.2. Most important symptoms/effects, acute and delayed

Symptoms/effects : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3. Indication of immediate medical attention and special treatment needed, if necessary

Other medical advice or treatment : Treat symptomatically.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

5.2. Specific hazards arising from the chemical

Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen chloride. Hydrogen fluoride.

Explosion hazard : Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers. May form flammable/explosive vapor-air mixture.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

Protection during firefighting : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

SECTION 6 Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe gas, fumes, vapor or spray.

For non-emergency personnel

Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

Emergency procedures : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level. Consider the risk of potentially explosive atmospheres. Eliminate every possible source of ignition.

Environmental precautions : Avoid release to the environment. Notify authorities if product enters sewers or public waters.

6.2. Methods and materials for containment and cleaning up

For containment : Stop leak if safe to do so. Dike for recovery or absorb with appropriate material.

Methods for cleaning up : Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.

Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

For further information refer to section 8: "Exposure controls/personal protection"

SECTION 7 Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe fumes, mist, spray, vapors. Wear personal protective equipment. Avoid contact with skin and eyes. Keep away from ignition sources (including static discharges). Proper grounding procedures to avoid static electricity should be followed. Use only non-sparking tools.

Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.

7.2. Conditions for safe storage, including incompatibilities

Technical measures : Comply with applicable regulations.

Storage conditions : Keep container closed when not in use. Keep away from ignition sources.

Storage area : Store in dry, cool, well-ventilated area.

Incompatible materials : Refer to Section 10 on Incompatible Materials.

SECTION 8 Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Appropiate engineering controls

Appropriate engineering controls : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

8.3. Individual protection measures, such as personal protective equipment

Hand protection:
protective gloves. 29 CFR 1910.138: Hand Protection
Eye protection:
Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection
Skin and body protection:
Wear suitable protective clothing
Respiratory protection:
In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection

Personal protective equipment symbol(s):

Other information:

Safety shoes. 29 CFR 1910.136: Foot Protection.

SECTION 9 Physical and chemical properties

9.1. Basic physical and chemical properties

Physical state	:	Liquid
Color	:	No data available
Odor	:	No data available
Odor threshold	:	No data available
pH	:	No data available
Melting point	:	-36 °C
Freezing point	:	No data available
Boiling point	:	138 – 139 °C
Flash point	:	47 °C
Flammability (solid, gas)	:	No data available
Vapor pressure	:	10.47 hPa (at 25 °C)
Relative vapor density at 20 °C	:	No data available
Relative density	:	No data available
Density	:	1.338 g/ml (@ 25 °C)
Molecular mass	:	180.56 g/mol
Solubility	:	Water: < 100 mg/l (at 23 °C)
Partition coefficient n-octanol/water (Log Pow)	:	3.7 (at 25 °C)
Auto-ignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, kinematic	:	No data available
Explosion limits	:	No data available
Particle characteristics	:	No data available

9.2. Data relevant with regard to physical hazard classes (supplemental)

Refractive index : 1.4444 (@ 25 °C)

SECTION 10 Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

The product is stable at normal handling and storage conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Keep away from heat, sparks and flame.

10.5. Incompatible materials

Strong bases. Strong oxidizing agents.

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

SECTION 11 Toxicological information

11.1. Likely routes of exposure

Acute toxicity (oral) : No data available
Acute toxicity (dermal) : No data available
Acute toxicity (inhalation) : No data available

4-Chlorobenzotrifluoride (98-56-6)	
LD50 oral rat	13 g/kg
LD50 dermal rabbit	> 2 ml/kg
LC50 Inhalation - Rat	33 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.

Serious eye damage/irritation : Causes serious eye irritation.

Respiratory or skin sensitization : May cause an allergic skin reaction.
Germ cell mutagenicity : No data available

Carcinogenicity : No data available

Reproductive toxicity : No data available
STOT-single exposure : May cause respiratory irritation.
STOT-repeated exposure : No data available
Aspiration hazard : No data available
Symptoms/effects : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

SECTION 12 Ecological information

12.1. Ecotoxicity

Hazardous to the aquatic environment, short–term (acute) : Toxic to aquatic life.

Hazardous to the aquatic environment, long–term (chronic) : Toxic to aquatic life with long lasting effects.

4-Chlorobenzotrifluoride (98-56-6)	
EC50 - Crustacea [1]	3.68 mg/l (Exposure time: 48 h - Species: Daphnia magna)

12.2. Persistence and degradability

4-Chlorobenzotrifluoride (98-56-6)	
Persistence and degradability	Rapidly degradable

12.3. Bioaccumulative potential

4-Chlorobenzotrifluoride (98-56-6)	
Partition coefficient n-octanol/water (Log Pow)	3.7 (at 25 °C)

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Ozone : No data available

Fluorinated greenhouse gases : No

SECTION 13 Disposal considerations

Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.

Product/Packaging disposal recommendations : Dispose of contents/container in accordance with licensed collector's sorting instructions.

Additional information : Recycle the material as far as possible.

SECTION 14 Transport information

14.1. UN number

UN-No.(DOT) : UN2234

UN-No. (TDG) : UN2234

UN-No. (IMDG) : 2234

UN-No. (IATA) : 2234

14.2. UN Proper Shipping Name

Proper Shipping Name (DOT) : Chlorobenzotrifluorides

Proper Shipping Name (TDG) : CHLOROBENZOTRIFLUORIDES

Proper Shipping Name (IMDG) : CHLOROBENZOTRIFLUORIDES

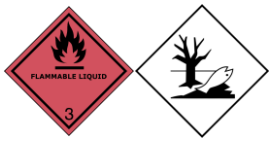
Proper Shipping Name (IATA) : Chlorobenzotrifluorides

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT) : 3

Hazard labels (DOT) : 3



TDG

Transport hazard class(es) (TDG) : 3

Hazard labels (TDG) : 3

IMDG

Transport hazard class(es) (IMDG) : 3

Hazard labels (IMDG) : 3

IATA

Transport hazard class(es) (IATA) : 3

Hazard labels (IATA) : 3

14.4. Packing group

Packing group (DOT) : III

Packing group (TDG) : III

Packing group (IMDG) : III

Packing group (IATA) : III

14.5. Environmental hazards

Dangerous for the environment : Yes

Marine pollutant : Yes

Other information : No supplementary information available.

14.6. Transport in bulk

Not applicable

14.7. Special precautions for user

DOT

UN-No.(DOT) : UN2234

DOT Special Provisions (49 CFR 172.102)	:	B1 - If the material has a flash point at or above 38 C (100 F) and below 93 C (200 F), then the bulk packaging requirements of 173.241 of this subchapter are applicable. If the material has a flash point of less than 38 C (100 F), then the bulk packaging requirements of 173.242 of this subchapter are applicable. IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). T2 - 1.5 178.274(d)(2) Normal..... 178.275(d)(3) TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = 97 / 1 + a (tr - tf) Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.
DOT Packaging Exceptions (49 CFR 173.xxx)	:	150
DOT Packaging Non Bulk (49 CFR 173.xxx)	:	203
DOT Packaging Bulk (49 CFR 173.xxx)	:	242
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	:	60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	:	220 L
DOT Vessel Stowage Location	:	A - The material may be stowed ‘‘on deck’’ or ‘‘under deck’’ on a cargo vessel and on a passenger vessel.
DOT Vessel Stowage Other	:	40 - Stow ‘‘clear of living quarters’’

TDG

UN-No. (TDG)	:	UN2234
Explosive Limit and Limited Quantity Index	:	5 L
Excepted quantities (TDG)	:	E1
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	:	60 L
Emergency Response Guide (ERG) Number	:	130

IMDG

Limited quantities (IMDG)	:	5 L
Excepted quantities (IMDG)	:	E1
Packing instructions (IMDG)	:	P001, LP01
IBC packing instructions (IMDG)	:	IBC03
Tank instructions (IMDG)	:	T2
Tank special provisions (IMDG)	:	TP1
EmS-No. (Fire)	:	F-E - FIRE SCHEDULE Echo - NON-WATER-REACTIVE FLAMMABLE LIQUIDS
EmS-No. (Spillage)	:	S-D - SPILLAGE SCHEDULE Delta - FLAMMABLE LIQUIDS
Stowage category (IMDG)	:	A
Stowage and handling (IMDG)	:	SW2
Segregation (IMDG)	:	SGG10
Flash point (IMDG)	:	36°C to 59°C c.c.
Properties and observations (IMDG)	:	Colourless liquids with an aromatic odour. Flashpoint: 36°C to 59°C c.c. On contact with moisture, can evolve hydrogen fluoride, which is a toxic and corrosive gas. Harmful by inhalation.

IATA

PCA Excepted quantities (IATA)	:	E1
PCA Limited quantities (IATA)	:	Y344
PCA limited quantity max net quantity (IATA)	:	10L
PCA packing instructions (IATA)	:	355
PCA max net quantity (IATA)	:	60L
CAO packing instructions (IATA)	:	366
CAO max net quantity (IATA)	:	220L
ERG code (IATA)	:	3L

SECTION 15 Regulatory information

15.1. Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

15.2. International regulations

CANADA

4-Chlorobenzotrifluoride (98-56-6)

Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

4-Chlorobenzotrifluoride (98-56-6)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations

4-Chlorobenzotrifluoride (98-56-6)

Listed introduction on Australian Industrial Chemicals Introduction Scheme (AICIS Inventory)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
Listed on the Japanese ENCS (Existing New Chemical Substances) inventory
Listed on the Japanese ISHL (Industrial Safety and Health Law)
Listed on KECL/KECI (Korean Existing Chemicals Inventory)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

15.3. State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16 Other information

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

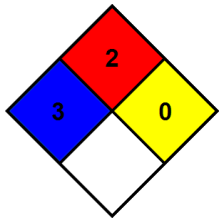
Revision date : 7/30/2026

Issue date : 12/17/2015

Full text of hazard classes and H-statements	
H226	Flammable liquid and vapor
H315	Causes skin irritation
H317	May cause an allergic skin reaction
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H401	Toxic to aquatic life
H411	Toxic to aquatic life with long lasting effects

NFPA health hazard : 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard	:	2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.
NFPA reactivity	:	0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health	:	2 Moderate Hazard - Temporary or minor injury may occur
Flammability	:	2 Moderate Hazard - Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F. (Classes II IIIA)
Physical	:	0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Safety Data Sheet (SDS), USA

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.