Material Safety Data Sheet
alpha,alpha,alpha-Trifluorotoluene, 99+%

ACC# 07328

Section 1 - Chemical Product and Company Identification

MSDS Name: alpha,alpha,alpha-Trifluorotoluene, 99+%
Catalog Numbers: AC139770000, AC139770050, AC139770500, AC139775000, AC9565018, AC9601208, AC9669161, XXAC13977-4L, XXAC13977-5G, XXAC1397723K
Synonyms: Benzotrifluoride; Phenylfluoroform; Toluene trifluoride.
Company Identification:

Fisher Scientific
1 Reagent Lane
Fair Lawn, NJ 07410

For information, call: 201-796-7100
Emergency Number: 201-796-7100
For CHEMTREC assistance, call: 800-424-9300
For International CHEMTREC assistance, call: 703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
98-08-8	Benzotrifluoride	> 99	202-635-0

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: clear colorless to slightly yellow liquid. Flash Point: 54 deg F.
Danger! Reacts with water to produce toxic and corrosive hydrogen fluoride. Corrosive. **Flammable liquid and vapor.** Causes respiratory tract irritation. May cause eye and skin irritation with possible burns. Causes severe digestive tract irritation with possible burns. May be harmful if swallowed, inhaled, or absorbed through the skin. Dangerous for the environment.
Target Organs: Central nervous system, eyes, skin, mucous membranes.

Potential Health Effects
Eye: Causes eye irritation. May cause chemical conjunctivitis and corneal damage.
Skin: Causes skin irritation. May cause irritation and dermatitis. May cause cyanosis of the extremities.
Ingestion: May cause gastrointestinal irritation with nausea, vomiting and diarrhea. May cause burns to the digestive tract. Ingestion of large amounts may cause CNS depression. Exposure to fluoride compounds can result in systemic toxic effects on the heart, liver, and kidneys. It may also deplete calcium levels in the body leading to hypocalcemia and death.
Inhalation: Causes respiratory tract irritation. Aspiration may lead to pulmonary edema. Vapors may cause dizziness or suffocation. Can produce delayed pulmonary edema. May cause burning sensation in the chest.
Chronic: Effects may be delayed. Chronic exposure to fluoride compounds may cause systemic toxicity.

Section 4 - First Aid Measures

Eyes: In case of contact, immediately flush eyes with plenty of water for a t least 15 minutes. Get medical aid immediately.
Skin: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Get medical aid immediately. Wash clothing before reuse.
Ingestion: If swallowed, do NOT induce vomiting. Get medical aid immediately. If victim is fully conscious, give a cupful of water. Never give anything by mouth to an unconscious person.
Inhalation: If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.
Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Flammable liquid and vapor. Vapors may be heavier than air. They can spread along the ground and collect in low or confined areas. Approach fire from upwind to avoid hazardous vapors and toxic decomposition products. Evacuate unnecessary personnel.
Extinguishing Media: For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Water may be ineffective. Do NOT get water inside containers. Reacts with water to produce toxic and corrosive hydrogen fluoride.
Flash Point: 54e deg F (12.22 deg C)
Autoignition Temperature: 1148 deg F (620.00 deg C)
Explosion Limits, Lower: Not available.
Upper: Not available.
NFPA Rating: (estimated) Health: 3; Flammability: 3; Instability: 1

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.
Spills/Leaks: Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Avoid runoff into storm sewers and ditches which lead to waterways. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. Do not get water inside containers. A vapor suppressing foam may be used to reduce vapors. Evacuate unnecessary personnel. Keep water away from spill to avoid hydrogen fluoride formation. Approach spill from upwind.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Do not get in eyes, on skin, or on clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Use with adequate ventilation. Wash clothing before reuse. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames. Avoid breathing vapor. Avoid use in confined spaces.
Storage: Keep away from heat, sparks, and flame. Keep away from sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area. Separate from oxidizing materials.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Use process enclosure, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Fluorides have TLV: TWA 2.5 mg/m3. Hydrogen fluoride (7664-39-3) has TLV: Ceiling 3 ppm.
Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Benzotrifluoride	none listed	none listed	none listed

OSHA Vacated PELs: Benzotrifluoride: No OSHA Vacated PELs are listed for this chemical.
Personal Protective Equipment
Eyes: Wear chemical goggles and a face shield.
Skin: Wear appropriate protective gloves to prevent skin exposure.
Clothing: Wear appropriate protective clothing to prevent skin exposure.
Respirators: A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

Section 9 - Physical and Chemical Properties

Physical State: Liquid
Appearance: clear colorless to slightly yellow
Odor: aromatic odor
pH: Not available.
Vapor Pressure: 31 mm Hg @ 20 deg C
Vapor Density: 5.03
Evaporation Rate: Not available.
Viscosity: Not available.
Boiling Point: 102 deg C
Freezing/Melting Point:-29 deg C
Decomposition Temperature: Not available.
Solubility: Reacts.
Specific Gravity/Density:1.19
Molecular Formula:C7H5F3
Molecular Weight:146.11

Section 10 - Stability and Reactivity

Chemical Stability: Reacts with water or moisture in air to form benzoic acid and hydrogen fluoride. Decomposition may release hydrogen fluoride.
Conditions to Avoid: Ignition sources, moisture, excess heat, electrical sparks, open flame.
Incompatibilities with Other Materials: Strong oxidizing agents, strong acids, strong bases.
Hazardous Decomposition Products: Carbon monoxide, irritating and toxic fumes and gases, carbon dioxide, hydrogen fluoride gas, organic fluorides.
Hazardous Polymerization: Has not been reported.

Section 11 - Toxicological Information

RTECS#:
CAS# 98-08-8: XT9450000
LD50/LC50:
CAS# 98-08-8:
Inhalation, mouse: LC50 = 92240 mg/m3/2H;
Inhalation, mouse: LC50 = 100000 mg/m3/2H;
Inhalation, rat: LC50 = 70810 mg/m3/4H;

Inhalation, rat: LC50 = 78100 mg/m3/4H;
Oral, mouse: LD50 = 10000 mg/kg;
Oral, mouse: LD50 = 10000 mg/kg;
Oral, rat: LD50 = 15 gm/kg;
Oral, rat: LD50 = 15000 mg/kg;
.
Dermal, rat: LD50 > 2000 mg/kg.
Carcinogenicity:
CAS# 98-08-8: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information available.
Teratogenicity: No information available.
Reproductive Effects: No information available.
Mutagenicity: No information available.
Neurotoxicity: No information available.
Other Studies:

Section 12 - Ecological Information

Ecotoxicity: Fish: Fathead Minnow: 12 mg/l; 96 hr; LC50Water flea Water Flea: 10 mg/l; 48 hr; EC50 No data available.
Environmental: If released to soil, benzotrifluoride will have low mobility. Biodegradation of benzotrifluoride will not be an important fate process in soil or water according to a biodegradation study. If released to water, benzotrifluoride may adsorb to suspended solids and sediment. Experimental results suggest that benzotrifluoride will bioconcentrate in aquatic organisms.
Physical: log Kow = 3.01
Other: No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.
RCRA P-Series: None listed.
RCRA U-Series: None listed.

Section 14 - Transport Information

	US DOT	Canada TDG
Shipping Name:	BENZOTRIFLUORIDE	BENZOTRIFLUORIDE
Hazard Class:	3	3
UN Number:	UN2338	UN2338
Packing Group:	II	II
Additional Info:		FLASHPOINT 12 C

Section 15 - Regulatory Information

US FEDERAL

TSCA
CAS# 98-08-8 is listed on the TSCA inventory.
Health & Safety Reporting List
None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules
None of the chemicals in this product are under a Chemical Test Rule.
Section 12b
None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule
None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs
None of the chemicals in this material have an RQ.
SARA Section 302 Extremely Hazardous Substances
None of the chemicals in this product have a TPQ.
Section 313 No chemicals are reportable under Section 313.
Clean Air Act:
This material does not contain any hazardous air pollutants.
This material does not contain any Class 1 Ozone depletors.
This material does not contain any Class 2 Ozone depletors.
Clean Water Act:
None of the chemicals in this product are listed as Hazardous Substances under the CWA.
None of the chemicals in this product are listed as Priority Pollutants under the CWA.
None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:
None of the chemicals in this product are considered highly hazardous by OSHA.
STATE
CAS# 98-08-8 can be found on the following state right to know lists: New Jersey, Pennsylvania, Massachusetts.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

F N

Risk Phrases:

R 11 Highly flammable.
R 51/53 Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Safety Phrases:

S 16 Keep away from sources of ignition - No smoking.
S 23 Do not inhale gas/fumes/vapour/spray.
S 61 Avoid release to the environment. Refer to special instructions /safety data sheets.

WGK (Water Danger/Protection)

CAS# 98-08-8: 1

Canada - DSL/NDSL

CAS# 98-08-8 is listed on Canada's NDSL List.

Canada - WHMIS

not available.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

Section 16 - Additional Information

MSDS Creation Date: 7/30/1999
Revision #4 Date: 10/03/2005