

2 HEALTH
3 FLAMMABILITY
1 PHYSICAL HAZARD

# MATERIAL SAFETY DATA SHEET

## Kowa American Corporation

CHEMTREC 24-HOUR EMERGENCY NUMBER (800) 424-9300

### SECTION 1

#### CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

**Product Name:**

**Benzotrifluoride  
[BTF]**

**Distributor's Name and Address  
in United States:**

Kowa American Corporation  
55 East 59<sup>th</sup> Street, 19<sup>th</sup> Floor  
New York, NY 10022  
Telephone: (212) 303-7800  
Facsimile: (212) 310-0101

**CHEMTREC 24-HOUR Emergency Number:**

**(800) 424-9300**

**Date Prepared:**

June 26, 2003  
[previous version: none]

### SECTION 2

#### COMPOSITION AND INFORMATION ON INGREDIENTS

Ingredient	CAS Registry No.	Weight %	Exposure Limits
Benzotrifluoride	98-08-8	99.5% (min.) 99.8% (typ.)	100 ppm TWA <sup>1</sup>
Water	7732-18-5	< 0.5 %	NE

#### Notes on Composition and Information on Ingredients

NE = Not established

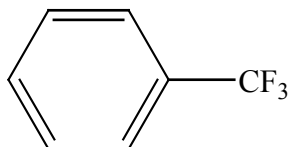
<sup>1</sup> The 100 ppm exposure limit is Kowa American's level for an 8-hour time weighted average. This 100 ppm limit is also the mandatory acceptable exposure limit (AEL) as required under the U.S. EPA's Significant New Alternatives Policy (SNAP) Program. See Section 15 of this MSDS for additional information.

## OTHER PRODUCT INFORMATION

**Chemical Name:** Benzene, (trifluoromethyl)- (9CI)

**Synonyms:** Toluene, .alpha.,.alpha.,.alpha.-trifluoro-  
Benzenyl fluoride  
Benzylidyne fluoride  
Phenylfluoroform

**Chemical Structure:**



**Molecular Formula:** C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>

**Molecular Weight:** 146.11

**EINECS No.:** 202-635-0

### SECTION 3 HAZARDS IDENTIFICATION

#### \*\*\*Emergency Overview\*\*\*

Water-white liquid with aromatic odor. Highly flammable. Keep container in a well ventilated place. Avoid all ignition sources. No smoking. May be slightly irritating to the skin, eyes, and respiratory system. Wear eye, skin, and respiratory protection. In case of contact with skin or eyes, rinse with water. Do not release to the environment – expected to be moderately toxic to aquatic organisms.

## POTENTIAL HEALTH EFFECTS

**EYES:** May be slightly irritating to the eyes. More serious effects may result if exposure is not treated. Vapors may irritate eyes.

**INHALATION:** Vapors may be slightly irritating to the upper respiratory tract (including nasal tissues). Prolonged exposure may be harmful and cause adverse effects including labored breathing and drowsiness, as well as damage to the upper respiratory tract and eyes.

**SKIN:** May be slightly irritating to the skin. The irritancy of this material varies from person to person. Exposure may also cause dermatitis due to defatting of the skin resulting in irritation, dryness, and cracking of the skin.

**INGESTION:** Oral toxicity of this material is low. Excessive exposure may cause liver, kidney, and/or thyroid damage.

**CHRONIC EFFECTS/CARCINOGENICITY:** Not regulated as a carcinogen. No long-term chronic effects or carcinogenicity data are known or available on this product.

NTP: *Not listed*

IARC: *Not listed*

OSHA: *Not listed*

**MUTAGENICITY:** This substance has generally produced negative results in *in vitro* mutagenicity tests.

**TERATOGENICITY (birth defects):** No teratogenic data are available on this material.

**REPRODUCTIVE TOXICITY:** Data on a structurally similar compound suggest that this substance is not expected to cause adverse reproductive effects.

**MEDICAL CONDITIONS AGGRAVATED BY EXPOSURE:** Chronic or overexposure may cause adverse effects in individuals with liver, kidney, or thyroid disorders.

**INCOMPATIBILITY:** Not known.

**SIGNS AND SYMPTOMS OF EXPOSURE:** Eye and respiratory tract irritation; labored breathing and drowsiness; loss of coordination possible if exposed to high concentrations. May cause defatting of the skin.

*See Section 11 – Toxicological Information for more information.*

<b>SECTION 4</b> <b>FIRST AID MEASURES</b>
---

## **FIRST AID MEASURES**

**SKIN:** Wash with plenty of water, then with soap and water for 15 minutes. Discard contaminated clothing and shoes. Call physician immediately if exposed to large quantities and/or if contact is prolonged.

**EYES:** Immediately flush with a continuous water stream for at least 20 minutes. Washing immediately after exposure is expected to be effective in preventing damage to the eyes. Get immediate medical attention.

**INHALATION:** Remove to fresh air. If not breathing give artificial respiration. If there is breathing difficulty, give oxygen. Get immediate medical attention.

**INGESTION/SWALLOWED:** Do not induce vomiting. Dilute by giving 1 or 2 glasses of milk or water. Nothing by mouth if unconscious. Get immediate medical attention.

## SECTION 5 FIRE FIGHTING MEASURES

**FLASH POINT:** 54 °F / 12 °C [closed cup]

**EXPLOSION/FLAMMABLE LIMITS:** Not known

**AUTOIGNITION TEMPERATURE:** > 650 °C

**EXTINGUISHING MEDIA:** Use dry chemical, foam, carbon dioxide, and water spray/fog as needed. For large fires alcohol resistant foams are preferred.

**SPECIAL FIRE FIGHTING PROCEDURES:** This material is highly flammable. As in any fire, wear a self-contained breathing apparatus pressure demand (MSHA/NIOSH approved or equivalent) and full protective gear. Toxic vapors, including hydrogen fluoride, may evolve. Fight fires from a safe distance or protected areas. Fire hoses with fog nozzles may be used for controlling fires but care must be exercised not to spread flaming. Use of large volumes of water may produce run-off that could be harmful to aquatic life and/or pose a hazardous waste disposal problem.

**UNUSUAL FIRE AND EXPLOSION HAZARDS:** This material is highly flammable. Sealed containers can explode in the heat of fire. Vapors may travel to ignition source because they are heavier than air. Run off may create an explosion, fire, and environmental hazard.

## SECTION 6 ACCIDENTAL RELEASE MEASURES

**SPILL/RELEASE AND CLEANUP PROCEDURES:** In case of spill, evacuate the area and remove all ignition sources. Dike and contain spill with vermiculite, clay-based absorbents, or other absorbent materials such as polyethylene fiber and polypropylene fiber products. Do not release to sewer systems; do not discharge the washings and other effluents into ponds, streams, or lakes. Wear appropriate respiratory and protective clothing as described in Section 8 during any cleanup and response activities. In the event of an uncontrolled release of this material, the user should determine if the release is reportable under applicable laws and regulations.

## SECTION 7 HANDLING AND STORAGE

**PRECAUTIONS TO BE TAKEN IN HANDLING AND STORAGE:** This material must be stored in an area free of heat and all ignition sources. Store in a cool dry place.

**OTHER PRECAUTIONS:** Do not drop. Keep away from fire, heat, open flames, lights, and all other ignition sources. Wear goggles and gloves when handling. Avoid breathing vapors. Eye-wash stations and emergency showers need to exist in areas where the material is handled, especially areas where loading and unloading operations occur. Wash hands thoroughly after handling and before eating, drinking, or smoking. Keep out of reach of children. Ground all containers when transferring the material.

Do not contaminate water, food, or feed by storage or disposal. Keep the product in original containers. Store in cool, dry, well ventilated, low fire risk area away from sunlight. Keep containers closed. Store only in approved containers, under approved conditions. Avoid pressure build-up in containers. An automatic water spray device should be immediately available. A spill control and containment plan should be provided. Storage area should not be subject to rapid temperature changes as such changes may cause increased internal pressure. Isolate from toxic materials or substances that may release corrosive, toxic, or flammable fumes on reaction.

## SECTION 8 EXPOSURE CONTROLS AND PERSONNEL PROTECTION

**RESPIRATORY PROTECTION:** Respirators equipped with organic vapor cartridges are anticipated to provide adequate respiratory protection during short-term exposures to low vapor concentrations of the material. Workers should wear a supplied-air respirator or self-contained breathing apparatus any time exposure is above low levels or during extended exposure periods. Use MSHA/NIOSH-approved respiratory equipment. Respirators should be selected based on the form and concentration of the contaminant in the air and in accordance with OSHA (29 CFR 1910.134). Handle only in the presence of adequate ventilation.

**PROTECTIVE GLOVES:** Wear chemical resistant gloves appropriate to the conditions to prevent skin exposure. Glove material comparisons indicate that gloves made of **NITRILE** are anticipated to afford adequate hand protection. (Gloves made of PVC, neoprene, and latex (natural rubber) are not expected to provide adequate hand protection.) Rinse and remove gloves immediately after use, and wash hands thoroughly with soap and water. Gloves should be removed and replaced immediately if there are any signs of degradation or breakthrough.

**PROTECTIVE CLOTHING:** Wear protective clothing and boots impervious to the product for the duration of the anticipated exposure if there is a potential for skin contact. An emergency shower should be readily accessible. Discard any contaminated clothing.

**EYE PROTECTION:** Chemical safety goggles meeting the specifications of ANSI Standard Z87.1 should be worn whenever there is the possibility of contact with the eyes. Spectacle type safety glasses do not provide satisfactory protection. An eyewash fountain should be readily accessible. Wear plastic face shield in addition to safety goggles where there is a danger of splashing.

**AIR MONITORING:** An air monitoring method has been partially validated for benzotrifluoride. Under this method, airborne concentrations of benzotrifluoride may be measured using SKC<sup>®</sup> 575 Series Passive Sampler badges. The sampling rate is 13.3 ml/minute with minimum and maximum sampling times of 15 minutes and 8 hours, respectively. The desorption efficiency is 106%. Analysis is conducted by gas chromatography with a flame ionization detector (GC/FID).

**EXPOSURE GUIDELINES:** Kowa American's exposure limit for an 8-hour time weighted average is 100 ppm. This 100 ppm limit is also the mandatory acceptable exposure limit (AEL) as required under the U.S. EPA's Significant New Alternatives Policy (SNAP) Program. See Section 15 of this MSDS for additional information.

## SECTION 9 PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance:</b>	Water white liquid
<b>Odor:</b>	Organic odor
<b>Boiling Point:</b>	102 °C (760 mm Hg)
<b>Specific Gravity:</b>	1.185 (20 °C)
<b>Density:</b>	9.9 lbs./gal.
<b>Vapor Pressure:</b>	32 mm Hg (20 °C) 40 mm Hg (25 °C) 127 mm Hg (50 °C) 321 mm Hg (75 °C)
<b>Vapor Density:</b>	5.0 (air = 1.0)
<b>Refractive Index (n<sub>D</sub>):</b>	1.41486 (13.3 °C)
<b>Melting Point:</b>	-29 °C
<b>Solubility in Water:</b>	450 mg/liter
<b>Other Solubility Information:</b>	<u>See</u> Note 1 below
<b>VOC Content:</b>	1,185 g/liter
<b>Volatile (%):</b>	100%

### Notes on Physical and Chemical Properties

<sup>1</sup>Benzotrifluoride is soluble in ethanol, benzene, ether, acetone, and n-heptane.

## SECTION 10 STABILITY AND REACTIVITY

**STABILITY:** Stable under normal conditions.

**CONDITIONS TO AVOID:** Avoid heat, fire, open flames, direct light, ignition sources, and UV radiation.

**INCOMPATIBILITY/MATERIALS TO AVOID:** Oxidizing and reducing agents.

**HAZARDOUS DECOMPOSITION OR BYPRODUCTS:** Not expected under normal conditions.

**HAZARDOUS POLYMERIZATION:** Hazardous polymerization will not occur.

<b>SECTION 11 TOXICOLOGICAL INFORMATION</b>
---

**ACUTE TOXICOLOGICAL DATA:**

Test	Result
Oral Rat LD <sub>50</sub>	15,000 mg/kg
Oral Mouse LD <sub>50</sub>	10,000 mg/kg
Dermal Rat LD <sub>50</sub>	> 2,000 mg/kg
Inhalation Rat LC <sub>50</sub>	50 - 80 mg/l [4-hour]
Inhalation Mouse LC <sub>50</sub>	90 - 100 mg/l [2-hour]
IP Mouse LD <sub>50</sub>	100 mg/kg

**EYE IRRITATION DATA:** This compound was found to be non-irritating to the eyes when tested in rabbits. The Draize values were reported to be 0.3/110 (washed) and 1.3/110 (unwashed).

**SKIN IRRITATION DATA:** This compound was found to be slightly irritating to the skin when tested in rabbits. The Draize value was reported to be 1.5/8.0.

**SKIN SENSITIZATION DATA:** No data are available.

**SUBCHRONIC DATA:** No data are available on this compound. A 13-week subchronic inhalation study on the structurally similar compound, *para*-chlorobenzotrifluoride (PCBTF), was conducted in rats exposed for 6 hours/day, 5 days/week at 0, 10, 51, or 252 ppm. An increase in liver weights was seen in the high dose group. No macroscopic effects were noted. No adverse central nervous system effects were observed as measured by motor activity, functional observation battery, or neuropathology. In a separate study on PCBTF, rats were dosed daily via oral gavage for three months at 0, 10, 40, 150, or 500 mg/kg. Effects noted included initial decrease in body weight gain, decreased food consumption, and changes in biochemical parameters. Increases were noted in liver, kidney, and thyroid weights in both sexes in most treatment groups. Microscopic effects were also observed in these same organs. No overt physical signs of toxicity were observed during treatment.

**REPRODUCTIVE TOXICITY:** No data are available on this compound. A two-generation reproduction study on the structurally similar compound, *para*-chlorobenzotrifluoride, was conducted in rats exposed daily via oral gavage at doses of 0, 5, 15, or 45 mg/kg. Only limited reproductive effects were noted.

**TERATOGENICITY (birth defects):** No data are available.

**MUTAGENICITY:** This substance has generally been found to be negative in the *in vitro* Ames test both with and without metabolic activation. Negative results have also been obtained in *in vitro* testing to assess DNA damage and repair. No *in vivo* mutagenicity data are available.

**CHRONIC EFFECTS/CARCINOGENICITY:** No data are available.

<b>SECTION 12</b> <b>ECOLOGICAL INFORMATION</b>
--

**SUMMARY OF ECOLOGICAL DATA:** Moderately toxic to aquatic organisms. Not expected to bioaccumulate. Biodegradation in water and soil is not anticipated since volatilization to the atmosphere is the principal fate process. Rapid volatilization is expected to occur from water surfaces. Expected to have low soil mobility. Atmospheric degradation is expected to readily occur. This substance is not an ozone-depleting substance.

**ECOTOXICOLOGICAL DATA:**

Test	Result
Fish LC <sub>50</sub> 96-hr	~ 20 mg/l
Daphnia LC <sub>50</sub> 48-hr	~ 10 mg/l
Algae EC <sub>50</sub> 24-hr	~ 20 mg/l

**ENVIRONMENTAL FATE DATA:** Testing and measured data show that this substance will not bioaccumulate in organisms; the BCF is estimated to be less than 100. Degradation is primarily expected to occur in the atmosphere; water and soil biodegradation is expected to be fair to poor.

**PHYSICAL/CHEMICAL PROPERTIES:** The measured Log K<sub>ow</sub> was found to be 3.01. The Henry's Law constant was determined to be 0.017 atm · m<sup>3</sup>/mole. The water solubility is 450 mg/l. The estimated k<sub>oc</sub> is estimated to be 1,030.

**SECTION 13  
DISPOSAL CONSIDERATIONS**

**RCRA CLASSIFICATION:** If discarded in its manufactured form, this product is a characteristic hazardous waste under RCRA. However, it is the responsibility of the user to determine at the time of disposal whether a material containing the product or derived from the product should be classified as a hazardous waste.

**SPECIAL INSTRUCTIONS:** Do not discharge or otherwise release this substance to sewer systems as flammable vapors may evolve into the available air-space and present a fire and/or explosion risk. Do not discharge effluent containing this product into any other bodies of water. This material is not soluble in water.

Large quantities of recovered benzotrifluoride should be considered for recycling due to the material's relative ease of distillation. All recovered material should be packaged, labeled, transported, and disposed in conformance with applicable laws and regulations. Incinerate the wastes in an approved facility that complies with local, state, and federal regulations. For disposing of the container, completely empty the container. Rinse empty container with water and dispose of the container in a sanitary landfill or by incineration.

**SECTION 14  
TRANSPORT INFORMATION**

**U.S./INTERNATIONAL SHIPPING INFORMATION UNDER DOT/IMO/IATA REGULATIONS:**

<b>Label/Placard:</b>	Flammable liquid
<b>Proper Shipping Name:</b>	Benzotrifluoride
<b>Hazard Class:</b>	Class 3, Packaging Group II
<b>UN or ID No.:</b>	UN 2338

Notes on Transport Information

None

**SECTION 15**  
**REGULATORY INFORMATION**

**REGULATORY STATUS:** This substance is listed on the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. This product, as well as its impurities, may trigger other specific reporting, recordkeeping, and testing requirements under: EPCRA/SARA III, RCRA, CERCLA, CAA, SDWA, and CWA.

**CLEAN AIR ACT STATUS:** Benzotrifluoride is identified as an acceptable substitute for ozone-depleting substances in the following three sectors: solvents, aerosols, and adhesives/coatings/inks. The compound is an acceptable substitute subject to a 100 ppm acceptable exposure limit. See EPA's June 8, 1999 Federal Register notice at 64 Fed. Reg. 30410 for more information.

**CALIFORNIA PROPOSITION 65:** This product contains no chemicals known to the State of California to cause cancer or reproductive toxicity.

**OTHER STATE CHEMICAL LISTS:** This product is identified on several state chemical lists including but not limited to Massachusetts, New Jersey, and Pennsylvania.

**SECTION 16**  
**OTHER INFORMATION**

**DISCLAIMER:** The information presented herein is believed to be factual. However, none of this information is to be taken as a warranty or representation for which Kowa American Corporation, its affiliates, the chemical manufacturer, or the preparer bears legal responsibility. The user should review any recommendation in the specific context of the intended use to determine whether it is appropriate.