



# TCI AMERICA

## SAFETY DATA SHEET

Revision number: 2  
Revision date: 10/06/2014

### 1. IDENTIFICATION

**Product name:** 3-Nitrobenzotrifluoride  
**Product code:** N0280

**Product use:** For laboratory research purposes.  
**Restrictions on use:** Not for drug or household use.

**Company:**  
TCI America  
9211 N. Harborage Street  
Portland, OR 97203 U.S.A.  
**Telephone:**  
+1-800-423-8616 / +1-503-283-1681  
**Fax:**  
+1-888-520-1075 / +1-503-283-1987  
**e-mail:**  
sales-US@TCIchemicals.com  
www.TCIchemicals.com

**Emergency telephone number:**  
**Chemical Emergencies:**  
TCI America (8:00am - 5:00pm) PST  
+1-503-286-7624  
**Transportation Emergencies:**  
Chemtrec 24-Hour  
+1-800-424-9300 (U.S.A.)  
+1-703-527-3887 (International)  
**Responsible department:**  
TCI America  
Environmental Health Safety and Security  
+1- 503-286-7624

### 2. HAZARD(S) IDENTIFICATION

**OSHA Haz Com: CFR 1910.1200:** Acute Toxicity - Oral [Category 4]  
Acute Toxicity - Inhalation [Category 2]  
Skin Corrosion/Irritation [Category 2]  
Eye Damage/Irritation [Category 2A]

**Signal word:** Danger!

**Hazard Statement(s):** Causes serious eye irritation  
Causes skin irritation  
Fatal if inhaled  
Harmful if swallowed

**Pictogram(s) or Symbol(s):**



**Precautionary Statement(s):**

**[Prevention]**

Do not eat, drink or smoke when using this product. Wash hands and face thoroughly after handling. Do not breathe fume, mist, vapors or spray. Use only outdoors or in a well-ventilated area. In case of inadequate ventilation wear respiratory protection. Wear protective gloves. Wear eye and face protection. If swallowed: Immediately call a poison center or doctor. Rinse mouth. If inhaled: Remove person to fresh air and keep comfortable for breathing. Immediately call a poison center or doctor. If on skin: Wash with plenty of water. If skin irritation or rash occurs: Get medical advice/attention. Take off contaminated clothing and wash it before reuse. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice or attention.

**[Response]**

**[Storage]**

**[Disposal]**

Store in a well-ventilated place. Keep container tightly closed. Store locked up.  
Dispose of contents and container in accordance with US EPA guidelines for the classification and determination of hazardous waste listed in 40 CFR 261.3. (See Section 13)

**3. COMPOSITION/INFORMATION ON INGREDIENTS**

<b>Substance/Mixture:</b>	Substance
<b>Components:</b>	3-Nitrobenzotrifluoride
<b>Percent:</b>	>96.0%(GC)
<b>CAS Number:</b>	98-46-4
<b>Molecular Weight:</b>	191.11
<b>Chemical Formula:</b>	C <sub>7</sub> H <sub>4</sub> F <sub>3</sub> NO <sub>2</sub>
<b>Synonyms:</b>	1-Nitro-3-(trifluoromethyl)benzene , 3-Nitro- $\alpha,\alpha,\alpha$ -trifluorotoluene

**4. FIRST-AID MEASURES**

<b>Inhalation:</b>	Immediately call a poison center or doctor. Move victim to fresh air. Give artificial respiration if victim is not breathing. Administer oxygen if breathing is difficult. Keep victim warm and quiet. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
<b>Skin contact:</b>	Immediately call a poison center or doctor. Remove and wash contaminated clothing before re-use. Remove and isolate contaminated clothing and shoes. In case of contact with substance, immediately flush skin with running water for at least 20 minutes. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
<b>Eye contact:</b>	IMMEDIATELY flush eyes with running water for at least 15 minutes, keeping eyelids open. Contact with material may irritate or burn eyes. Call emergency medical service. Move victim to fresh air. Check for and remove any contact lenses. Keep victim warm and quiet. Treat symptomatically and supportively. Effects of exposure to substance may be delayed. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
<b>Ingestion:</b>	Harmful if swallowed. Do not induce vomiting without medical advice. Call a physician or Poison Control Center immediately. Do not use mouth-to-mouth method if victim ingested the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Loosen tight clothing such as a collar, tie, belt or waistband. If a person vomits place them in the recovery position so that vomit will not reenter the mouth and throat. Rinse mouth. Keep victim warm and quiet. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
<b>Symptoms/effects:</b>	
<b>Acute:</b>	Redness.
<b>Delayed:</b>	No data available

<b>Immediate medical attention:</b>	WARNING: It might be dangerous to the person providing aid to give mouth-to-mouth respiration, because the inhaled material is toxic. If breathing has stopped, perform artificial respiration. Use first aid treatment according to the nature of the injury. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.
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**5. FIRE-FIGHTING MEASURES**

<b>Suitable extinguishing media:</b>	Dry chemical, CO <sub>2</sub> or water spray. Consult with local fire authorities before attempting large scale fire fighting operations.
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**Specific hazards arising from the chemical**

<b>Hazardous combustion products:</b>	These products include: Carbon oxides Nitrogen oxides Halogenated compounds
<b>Other specific hazards:</b>	WARNING: Highly toxic HF gas is produced during combustion.

**Special precautions for fire-fighters:**

Use water spray or fog; do not use straight streams. Dike fire-control water for later disposal; do not scatter the material. Containers may explode when heated. Move containers from fire area if you can do it without risk.

**Special protective equipment for fire-fighters:**

Wear positive pressure self-contained breathing apparatus (SCBA). Structural fire fighters' protective clothing provides limited protection in fire situations ONLY; it may not be effective in spill situations. Wear chemical protective clothing which is specifically recommended by the manufacturer. It may provide little or no thermal protection.

**6. ACCIDENTAL RELEASE MEASURES**

<b>Personal precautions:</b>	Avoid contact with skin, eyes, and clothing. Keep people away from and upwind of spill/leak. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing (Section 8). Warn unnecessary personnel to move away. Stop leak if you can do it without risk. Ensure adequate ventilation. Isolate the hazard area and deny entry to unnecessary and unprotected personnel.
<b>Personal protective equipment:</b>	Wear eye protection (splash goggles) and face protection (full length face shield). Lab coat. Vapor respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent. Wear protective gloves (nitrile).

**6. ACCIDENTAL RELEASE MEASURES**

**Emergency procedures:** In case of a spill and/or a leak, always shut off any sources of ignition, ventilate the area, and exercise caution. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Warn personnel to move away. Prevent entry into sewers, basements or confined areas; dike if needed.

**Methods and materials for containment and cleaning up:**

ELIMINATE all ignition sources (no smoking, flares, sparks, or flames in immediate area). Stop leak if without risk. Ventilate the area. Absorb with an inert material and put the spilled material in an appropriate waste disposal container. Use clean non-sparking tools to collect absorbed material.

**Environmental precautions:**

Keep away from living quarters. Prevent further leakage or spillage if safe to do so. Water runoff can cause environmental damage. Prevent entry into sewers, basements or confined areas; dike if needed.

**7. HANDLING AND STORAGE**

**Precautions for safe handling:** Do NOT breath gas, fumes, vapor, or spray. Do not ingest. Avoid contact with skin and eyes. Good general ventilation should be sufficient to control airborne levels. Keep container dry. Handle and open container with care. Wear suitable protective clothing, gloves and eye/face protection. When using do not eat, drink, or smoke. Keep away from sources of ignition.

**Conditions for safe storage:** Store locked up. Keep containers tightly closed in a cool, well-ventilated place. Keep away from incompatibles. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Avoid prolonged storage periods.

**Storage incompatibilities:** Store away from oxidizing agents

**8. EXPOSURE CONTROLS / PERSONAL PROTECTION**

**Exposure limits:** No data available

**Appropriate engineering controls:**

Good general ventilation should be sufficient to control airborne levels. Ventilation is normally required when handling or using this product. Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substance. Follow safe industrial engineering/laboratory practices when handling any chemical.

**Personal protective equipment**

**Respiratory protection:** Vapor respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent.

**Hand protection:** Wear protective gloves.

**Eye protection:** Splash goggles.

**Skin and body protection:** Lab coat.

**9. PHYSICAL AND CHEMICAL PROPERTIES**

**Physical state (20°C):** Liquid  
**Form:** Clear  
**Color:** Very pale yellow - Yellow  
**Odor:** No data available  
**Odor threshold:** No data available

**Melting point/freezing point:** No data available

**Boiling point/range:** 203°C (397°F)

**Decomposition temperature:** No data available

**Relative density:** 1.43

**Kinematic Viscosity:** No data available

**Partition coefficient:  
n-octanol/water (log P<sub>ow</sub>)** No data available

**Flash point:** 103°C (217°F)

**Flammability (solid, gas):** No data available

**pH:** No data available

**Vapor pressure:** No data available

**Vapor density:** No data available

**Dynamic Viscosity:** No data available

**Evaporation rate:  
(Butyl Acetate = 1)** No data available

**Autoignition temperature:** No data available

**Flammability or explosive limits:**

**Lower:** No data available

**Upper:** No data available

**Solubility(ies):**

**10. STABILITY AND REACTIVITY**

**Reactivity:** Not Available.

**Chemical Stability:** Stable under recommended storage conditions. (See Section 7)

**Possibility of Hazardous Reactions:** No hazardous reactivity has been reported.

**10. STABILITY AND REACTIVITY**

<b>Conditions to avoid:</b>	Avoid excessive heat and light.
<b>Incompatible materials:</b>	Alkali, Bases, Reducing agents, Strong oxidizing agents
<b>Hazardous Decomposition Products:</b>	No data available

**11. TOXICOLOGICAL INFORMATION**

**RTECS Number:** XT3500000

**Acute Toxicity:**

ipr-mus LD50:100 mg/kg

ori-rat LD50:610 mg/kg

**Skin corrosion/irritation:**

No data available

**Serious eye damage/irritation:**

No data available

**Respiratory or skin sensitization:**

No data available

**Germ cell mutagenicity:**

No data available

**Carcinogenicity:**

No data available

**IARC:** No data available

**NTP:** No data available

**OSHA:** No data available

**Reproductive toxicity:**

No data available

**Routes of Exposure:**

Inhalation, Eye contact, Ingestion, Skin contact.

**Symptoms related to exposure:**

Overexposure may result in serious illness or death. Skin contact may result in inflammation; characterized by itching, scaling, reddening, or occasionally blistering. Skin contact may result in redness, pain or dry skin. Eye contact may result in redness or pain.

**Potential Health Effects:**

Skin and eye contact may result in irritation.

**Target organ(s):**

No data available

**12. ECOLOGICAL INFORMATION****Ecotoxicity**

<b>Fish:</b>	No data available
<b>Crustacea:</b>	No data available
<b>Algae:</b>	No data available

**Persistence and degradability:**

No data available

**Bioaccumulative potential (BCF):**

No data available

**Mobility in soil:**

No data available

**Partition coefficient:**

No data available

**n-octanol/water (log P<sub>ow</sub>)****Soil adsorption (K<sub>oc</sub>):**

No data available

**Henry's Law:**

No data available

**constant (PaM<sup>3</sup>/mol)****13. DISPOSAL CONSIDERATIONS****Disposal of product:**

Recycle to process if possible. It is the generator's responsibility to comply with Federal, State and Local rules and regulations. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. This section is intended to provide assistance but does not replace these laws, nor does compliance in accordance with this section ensure regulatory compliance according to the law. US EPA guidelines for Identification and Listing of Hazardous Waste are listed in 40 CFR Parts 261. The product should not be allowed to enter the environment, drains, water ways, or the soil.

**13. DISPOSAL CONSIDERATIONS**

**Disposal of container:** Dispose of as unused product. Do not re-use empty containers.  
**Other considerations:** Observe all federal, state and local regulations when disposing of the substance.

**14. TRANSPORT INFORMATION****DOT (US)**

<b>UN number:</b> UN2306	<b>Proper Shipping Name:</b> Nitrobenzotrifluorides, liquid	<b>Class or Division:</b> 6.1 Toxic material.	<b>Packing Group:</b> II
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**IATA**

<b>UN number:</b> UN2306	<b>Proper Shipping Name:</b> Nitrobenzotrifluorides, liquid	<b>Class or Division:</b> 6.1 Toxic material.	<b>Packing Group:</b> II
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**IMDG**

<b>UN number:</b> UN2306	<b>Proper Shipping Name:</b> Nitrobenzotrifluorides, liquid	<b>Class or Division:</b> 6.1 Toxic material.	<b>Packing Group:</b> II
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**Marine Pollutant:** Marine Pollutant  
**EmS number:** F-A, S-A

**15. REGULATORY INFORMATION****Toxic Substance Control Act (TSCA 8b.):**

This product is ON the EPA Toxic Substances Control Act (TSCA) inventory.

**US Federal Regulations****CERCLA Hazardous substance and Reportable Quantity:**

<b>SARA 313:</b>	Not Listed
<b>SARA 302:</b>	Not Listed

**State Regulations****State Right-to-Know**

<b>Massachusetts</b>	Not Listed
<b>New Jersey</b>	Listed
<b>Pennsylvania</b>	Not Listed
<b>California Proposition 65:</b>	Not Listed

**Other Information****NFPA Rating:**

<b>Health:</b>	4
<b>Flammability:</b>	2
<b>Instability:</b>	0

**HMIS Classification:**

<b>Health:</b>	4
<b>Flammability:</b>	2
<b>Physical:</b>	0

**International Inventories**

**WHMIS hazard class:** D1A: Materials causing immediate and serious toxic effects. (Very Toxic)  
D2A: Materials causing other toxic effects. (Very Toxic)  
D2B: Materials causing other toxic effects. (Toxic)  
**EC-No:** 202-670-1

**16. OTHER INFORMATION**

**Revision date:** 10/06/2014  
**Revision number:** 2

**16. OTHER INFORMATION**

TCI chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its affiliates or subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our SDS are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated SDS for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, face mask, fume hood). For proper handling and disposal, always comply with federal, state and local regulations.