

## Chemical Safety Data Sheet MSDS / SDS

## 4-Nitrobenzotrifluoride

Revision Date:2024-12-21 Revision Number:1

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

**Product identifier**

Product name : 4-Nitrobenzotrifluoride  
CBnumber : CB9346938  
CAS : 402-54-0  
EINECS Number : 206-948-3  
Synonyms : 1-nitro-4-(trifluoromethyl)benzene,4-Nitrobenzotrifluoride

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

## SECTION 2: Hazards identification

**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral  
Skin irritation, Category 2  
Eye irritation, Category 2  
Acute toxicity - Category 2, Inhalation  
Specific target organ toxicity – single exposure, Category 3

**Label elements****Pictogram(s)**

□

Signal word : Danger

**Hazard statement(s)**

H301 Toxic if swallowed  
H302 Harmful if swallowed  
H311 Toxic in contact with skin  
H315 Causes skin irritation

H319 Causes serious eye irritation

H330 Fatal if inhaled

H335 May cause respiratory irritation

#### **Precautionary statement(s)**

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P284 Wear respiratory protection.

P310 Immediately call a POISON CENTER or doctor/physician.

P320 Specific treatment is urgent (see ... on this label).

P330 Rinse mouth.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position 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.

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P405 Store locked up.

#### **Prevention**

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

#### **Response**

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P320 Specific treatment is urgent (see ... on this label).

P319 Get medical help if you feel unwell.

#### **Storage**

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

#### **Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

#### **Other hazards**

no data available

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 4-Nitrobenzotrifluoride
Synonyms	: 1-nitro-4-(trifluoromethyl)benzene,4-Nitrobenzotrifluoride
CAS	: 402-54-0
EC number	: 206-948-3
MF	: C7H4F3NO2
MW	: 191.11

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## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Highly toxic, may be fatal if inhaled, swallowed or absorbed through skin. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

### Indication of any immediate medical attention and special treatment needed

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: SMALL FIRE: Dry chemical, CO<sub>2</sub> or water spray. LARGE FIRE: Water spray, fog or regular foam. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. Use water spray or fog; do not use straight streams. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay

away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

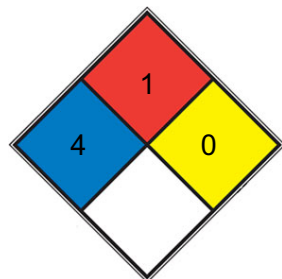
### Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Combustible material: may burn but does not ignite readily. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### NFPA 704



**HEALTH 4** Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, [hydrofluoric acid](#))

**FIRE 1** Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

**SPEC.**  
**HAZ.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

## SECTION 7: Handling and storage

### Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	Crystalline Powder, Crystals or Crystalline Mass
Colour	White to yellow
Odour	no data available
Melting point/freezing point	-70°C(lit.)
Boiling point or initial boiling point and boiling range	82°C/10mmHg(lit.)
Flammability	no data available

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Lower and upper explosion limit/flammability limit	no data available
Flash point	89°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	0.454mmHg at 25°C
Density and/or relative density	1.417g/cm <sup>3</sup>
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

Organonitrate compounds range from slight to strong oxidizing agents. If mixed with reducing agents, including hydrides, sulfides and nitrides, they may begin a vigorous reaction that culminates in a detonation. The aromatic nitro compounds may explode in the presence of a base such as sodium hydroxide or potassium hydroxide even in the presence of water or organic solvents. The explosive tendencies of aromatic nitro compounds are increased by the presence of multiple nitro groups.

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available

- Dermal: no data available

**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

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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## SECTION 12: Ecological information

**Toxicity**

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

**Persistence and degradability**

no data available

**Bioaccumulative potential**

no data available

**Mobility in soil**

no data available

## Other adverse effects

no data available

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## SECTION 13: Disposal considerations

### Disposal methods

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### UN Number

ADR/RID: UN3431 (For reference only, please check.)

IMDG: UN3431 (For reference only, please check.)

IATA: UN3431 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: NITROBENZOTRIFLUORIDES, SOLID (For reference only, please check.)

IMDG: NITROBENZOTRIFLUORIDES, SOLID (For reference only, please check.)

IATA: NITROBENZOTRIFLUORIDES, SOLID (For reference only, please check.)

### Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

### Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (For reference only, please check.)

### Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

### Special precautions for user



no data available

### **Transport in bulk according to IMO instruments**

no data available

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## SECTION 15: Regulatory information

### **Safety, health and environmental regulations specific for the product in question**

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

#### **EC Inventory**

Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Not Listed.

#### **China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

#### **PICCS**

Not Listed.

#### **Vietnam National Chemical Inventory**

Listed.

#### **IECSC**

Not Listed.

#### **Korea Existing Chemicals List (KECL)**

Not Listed.

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## SECTION 16: Other information

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### **References**

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pagelD=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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