

## Chemical Safety Data Sheet MSDS / SDS

## Benzotrifluoride

Revision Date:2024-05-11 Revision Number:1

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

## Product identifier

Product name : Benzotrifluoride  
CBnumber : CB1292738  
CAS : 98-08-8  
EINECS Number : 202-635-0  
Synonyms : BENZOTRIFLUORIDE, $\alpha,\alpha,\alpha$ -trifluorotoluene

## 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

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P201 Obtain special instructions before use.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P308+P313 IF exposed or concerned: Get medical advice/attention.  
P370+P378 In case of fire: Use ... for extinction.

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

P403+P235 Store in a well-ventilated place. Keep cool.

#### **Hazard statements**

H225 Highly Flammable liquid and vapour

H304 May be fatal if swallowed and enters airways

H315 Causes skin irritation

H319 Causes serious eye irritation

H331 Toxic if inhaled

H340 May cause genetic defects

H350 May cause cancer

H351 Suspected of causing cancer

H370 Causes damage to organs

H372 Causes damage to organs through prolonged or repeated exposure

H401 Toxic to aquatic life

H411 Toxic to aquatic life with long lasting effects

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## SECTION 3: Composition/information on ingredients

### **Substance**

|              |  |
|--------------|--|
| Product name | : Benzotrifluoride   |
| Synonyms     | : BENZOTRIFLUORIDE, $\alpha,\alpha,\alpha$ -trifluorotoluene |
| CAS          | : 98-08-8  |
| EC number    | : 202-635-0  |
| MF           | : C7H5F3   |
| MW           | : 146.11   |

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

After inhalation: fresh air.

#### **In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### **In case of eye contact**

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### **If swallowed**

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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

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

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

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

Foam Water

### Special hazards arising from the substance or mixture

Carbon oxides Hydrogen fluoride Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors. Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

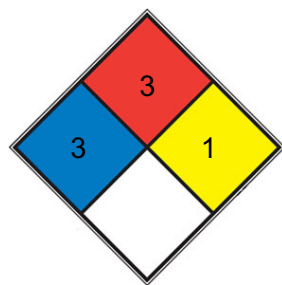
### Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

■ REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

□ SPEC.

□ HAZ.

## SECTION 6: Accidental release measures

### **Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### **Environmental precautions**

Do not let product enter drains. Risk of explosion.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb? ). Dispose of properly. Clean up affected area.

### **Reference to other sections**

For disposal see section 13.

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## SECTION 7: Handling and storage

### **Precautions for safe handling**

### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

### **Hygiene measures**

Change contaminated clothing. Wash hands after working with substance. For precautions see section 2.2.

### **Conditions for safe storage, including any incompatibilities**

### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

### **Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### **control parameter**

### **Hazard composition and occupational exposure limits**

Does not contain substances with occupational exposure limits.

### **Exposure controls**

## Personal protective equipment

### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other

substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact Material: Viton?

Minimum layer thickness: 0,7 mm Break through time: 480 min

Material tested: Vitoject? (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 120 min

Material tested: Camatril? (KCL 730 / Aldrich Z677442, Size M)

### Body Protection

Flame retardant antistatic protective clothing.

### Respiratory protection

required when vapours/aerosols are generated. Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|  |  |
|--|--|
| Appearance                                   | colorless clear, liquid                                      |
| Odour  | No data available  |
| Odour Threshold                              | No data available  |
| pH   | No data available  |
| Melting point/freezing point                 | Melting point/range: -29 °C - lit.                           |
| Initial boiling point and boiling range      | 102 °C - lit.  |
| Flash point                                  | 8 °C - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| Evaporation rate                             | No data available  |
| Flammability (solid, gas)                    | No data available  |
| Upper/lower flammability or explosive limits | 1.4-9.3%(V)  |

|  |   |
|--|---|
| Vapour pressure                        | 69,99 hPa at 20 °C - OECD Test Guideline 104  |
| Vapour density                         | 5,04 - (Air = 1.0)  |
| Relative density                       | 1.199   |
| Water solubility                       | 0,151 g/l at 20 °C - OECD Test Guideline 105  |
| Partition coefficient: n-octanol/water | Pow: 1.031; log Pow: 3,01 at 20 °C - OECD Test Guideline 117 - Bioaccumulation is not expected. |
| Autoignition temperature               | not auto-flammable  |
| Decomposition temperature              | No data available   |
| Viscosity                              | Viscosity, kinematic: No data available Viscosity, dynamic: No data available                   |
| Explosive properties                   | No data available   |
| Oxidizing properties                   | No data available   |

### Other safety information

Relative vapor density

5,04 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### Reactivity

Vapors may form explosive mixture with air.

### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### Possibility of hazardous reactions

Generates dangerous gases or fumes in contact with: Water

Violent reactions possible with:

Strong oxidizing agents strong reducing agents Strong bases

### Conditions to avoid

Warming.

### Incompatible materials

No data available

### Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Mouse - 10.000 mg/kg Remarks: Behavioral:General anesthetic. Behavioral:Excitement.

Behavioral: Muscle weakness.

LC50 Inhalation - Rat - 4 h - 70.810 mg/m<sup>3</sup> LD50 Dermal - Rat - > 2.000 mg/kg

(OECD Test Guideline 402)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation - 72 h (OECD Test Guideline 405)

#### **Respiratory or skin sensitization**

(OECD Test Guideline 442C)

#### **Germ cell mutagenicity**

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung (CHL/IU) cells

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan)

Metabolic activation: with and without metabolic activation

Result: Negative

Test Type: Ames test

Test system: Salmonella typhimurium TA100, TA1535, TA98, TA1537, Escherichia coli WP2 uvrA

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD (471 and 472)

Metabolic activation: with and without metabolic activation

Result: Negative

#### **Carcinogenicity**

No data available

#### **Reproductive toxicity**

No data available

#### **Specific target organ toxicity - single exposure**

No data available

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

#### **Toxicity**

LD50 orally in Rabbit: 15000 mg/kg LD50 dermal Rat > 2000 mg/kg

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## SECTION 12: Ecological information

### **Toxicity**

#### **Toxicity to fish**

LC50 - Oryzias latipes - 19,4 mg/l - 96 h Remarks: (ECHA)

#### **Toxicity to daphnia and other aquatic invertebrates**

semi-static test EC50 - Daphnia magna (Water flea) - 3,11 mg/l - 48 h

(OECD Test Guideline 202)

#### **Toxicity to algae**

static test EC50 - Pseudokirchneriella subcapitata - 5,4 mg/l - 72 h (OECD Test Guideline 201)

#### **Toxicity to bacteria**

EC5 - activated sludge - 10 - 100 mg/l - 24 h

Remarks: (IUCLID)

#### **Persistence and degradability**

Biodegradability aerobic - Exposure time 28 d

Result: 74 % - Not readily biodegradable. (OECD Test Guideline 301D)

#### **Bioaccumulative potential**

No data available

#### **Mobility in soil**

No data available

#### **Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### **Other adverse effects**

Biological effects:

Forms toxic and corrosive mixtures with water even if diluted. Possible decomposition products in case of hydrolysis are: Hydrogen fluoride

Further information on ecology

Discharge into the environment must be avoided.

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## SECTION 13: Disposal considerations

#### **Waste treatment methods**

#### **Product**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

#### **UN number**

ADR/RID: 2338 IMDG: 2338 IATA: 2338

#### **UN proper shipping name**



ADR/RID: BENZOTRIFLUORIDE

IMDG: BENZOTRIFLUORIDE

IATA: Benzotrifluoride

### **Transport hazard class(es)**

ADR/RID: 3 IMDG: 3 IATA: 3

### **Packaging group**

ADR/RID: II IMDG: II IATA: II

### **Environmental hazards**

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

### **Special precautions for user**

No data available

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## SECTION 15: Regulatory information

### **Safety, health and environmental regulations/legislation specific for the substance or mixture**

#### **Regulations on the Safety Management of Hazardous Chemicals**

China Catalog of Hazardous chemicals 2015:Listed. website: <https://www.mem.gov.cn/>

#### **Measures for Environmental Management of New Chemical Substances**

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

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## SECTION 16: Other information

### **Abbreviations and acronyms**

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

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