

## Chemical Safety Data Sheet MSDS / SDS

**3-Aminobenzotrifluoride**

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

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 3-Aminobenzotrifluoride  
CBnumber : CB8854748  
CAS : 98-16-8  
EINECS Number : 202-643-4  
Synonyms : 3-(trifluoromethyl)aniline,3-Aminobenzotrifluoride

**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**

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P264 Wash hands thoroughly after handling.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P284 Wear respiratory protection.  
P302+P352 IF ON SKIN: wash with plenty of soap and water.

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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P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

P391 Collect spillage. Hazardous to the aquatic environment

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

P405 Store locked up.

P501 Dispose of contents/container to.....

#### **Hazard statements**

H227 Combustible liquid

H302 Harmful if swallowed

H312 Harmful in contact with skin

H315 Causes skin irritation

H319 Causes serious eye irritation

H330 Fatal if inhaled

H373 May cause 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	: 3-Aminobenzotrifluoride
Synonyms	: 3-(trifluoromethyl)aniline,3-Aminobenzotrifluoride
CAS	: 98-16-8
EC number	: 202-643-4
MF	: C7H6F3N
MW	: 161.12

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## SECTION 4: First aid measures

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

#### **General advice**

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

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

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

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

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

Flush eyes with water as a precaution.

#### **If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

## 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

Small (incipient) fires must be extinguished with alcohol resistant foam, dry chemical powder or carbon dioxide. Large amounts of water are ineffective. Cool containers with large amounts of water.

#### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride

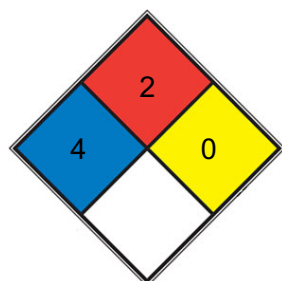
#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### Further information

Use water spray to cool unopened containers.

#### NFPA 704



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

**FIRE 2** Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

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

SPEC.

HAZ.

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## SECTION 6: Accidental release measures

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

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

## **Environmental precautions**

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

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet- brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

## **Reference to other sections**

For disposal see section 13.

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# SECTION 7: Handling and storage

## **Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

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

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

## **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**

### **Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### **Personal protective equipment**

#### **Eye/face protection**

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

#### **Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

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

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

Splash contact

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

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

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

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

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	light brown clear, liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 5 - 6 °C - lit.
Initial boiling point and boiling range	187 °C - lit.
Flash point	87 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0.3 mm Hg ( 20 °C)
Vapour density	No data available
Relative density	1,29 g/cm <sup>3</sup> at 25 °C

Water solubility	5 g/L (20°C)
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat, flames and sparks.

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 480 mg/kg

LD50 Dermal - Rabbit - 1.330 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). Lungs, Thorax, or Respiration:Dyspnea. Prolonged skin contact may cause skin irritation and/or dermatitis.

#### Skin corrosion/irritation

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

May cause damage to organs through prolonged or repeated exposure.

**Aspiration hazard**

No data available

**Additional Information**

RTECS: XU9180000

Cough, Shortness of breath, Headache, Nausea, Vomiting, May cause cyanosis., prolonged or repeated exposure can cause:, Dizziness

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## SECTION 12: Ecological information

**Toxicity**

No data available

**Toxicity to daphnia and other aquatic invertebrates**

EC50 - Daphnia magna (Water flea) - 2,7 mg/l - 48 h

**Persistence and degradability**

No data available

**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**

Toxic to aquatic life. No data available

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## SECTION 13: Disposal considerations

### Waste treatment methods

#### Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Incompatibilities

Incompatible with oxidizers (chlorates, nitrates, peroxides, permanganates, perchlorates, chlorine, bromine, fluorine, etc.); contact may cause fires or explosions. Keep away from alkaline materials, strong bases, strong acids, oxoacids, epoxides. Light and air sensitive.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### UN number

ADR/RID: 2948 IMDG: 2948 IATA: 2948

### UN proper shipping name

	ADR/RID: 3-TRIFLUOROMETHYLANILINE IMDG: 3-TRIFLUOROMETHYLANILINE	
	IATA: 3-Trifluoromethylaniline	
14.3	Transport hazard class(es) ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group ADR/RID: II IMDG: II	IATA: II
14.5	Environmental hazards ADR/RID: no IMDG Marine pollutant: no	IATA: no
14.6	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

EC Inventory:Listed.

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

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

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



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

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

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

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

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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

【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:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.