

## 1: Identification of substance / mixture

### 1. Product Identifier

Substance

Product Name **3-Aminobenzotrifluoride**  
Product Code 001602  
CAS Number 98-16-8  
Other Names  
IUPAC  
MFCD Number MFCD00007797  
EC/EINECS 202-643-4  
REACH Number

### 2. Relevant identified uses of the substance or mixture and uses advised against

Research and Development

### 3. Details of the supplier of the safety data sheet

Fluorochem Ltd  
Unit 14, Graphite Way  
Hadfield  
Derbyshire  
SK13 1QH  
UK

Telephone: +44(0)1457 860111  
Fax: +44(0)1457 892799  
Email: sds@fluorochem.co.uk



### 4. Emergency telephone number

+44(0)7855 268577 -

## 2. Hazards Identification

### 1. Classification of the substance or mixture

H302	Acute Tox. 4	R22, R20/22, R20/21/22, R21/22, R68/20/22, R68/21/22, R68/20/21/22
H315	Skin Irrit. 2	R38, R36/38, R36/37/38, R37/38
H319	Eye Irrit. 2	R36, R36/37, R36/38, R36/37/38
H330	Acute Tox. 2	R23, R26, R26, R26/27, R26/27, R26/27/28, R26/27/28, R26/28, R26/28, R23/24, R23/24/25, R23/25, R23/34/35
H373	STOT RE 2	R33, R48/20, R48/21, R48/22, R48/20/21, R48/20/22, R48/21/22, R48/20/21/22

No Resource File

### 2. Label elements

Signal Word **Danger**



### Hazard Statements

H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H373	May cause damage to organs ..

### Precautionary Phrases

P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

### 3. Other Hazards

Additional precautionary phrases are located throughout the safety data sheet

## 3. Composition / Information on Ingredients

## 1. Substances

3-Aminobenzotrifluoride

Assay:100% CAS Number :98-16-8

## 2. Mixtures

Not Relevant

## 4. First Aid Measures

### 1. Description of first aid measures

<i>Skin Contact</i>	P302 + P352: IF ON SKIN: Wash with plenty of soap and water. Wash immediately with plenty of soap and water. Transfer to hospital if there are burns or symptoms of poisoning.
<i>Eye Contact</i>	Rinse opened eye for several minutes under running water. Transfer to hospital for specialist examination.
<i>Ingestion</i>	Wash out mouth with water. Transfer to hospital as soon as possible.
<i>Inhalation</i>	P304 + P340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Supply fresh air; consult a doctor in case of complaints. Transfer to hospital as soon as possible.

### 2. Most important symptoms and effects

There may be pain and redness.  
May cause permanent damage.  
There may be difficulty swallowing.

### 3. Indication of any immediate medical attention

No additional measures required

## 5. Firefighting measures

### 1. Extinguishing Media

<i>Suitable</i>	Carbon dioxide. Alcohol resistant foam. Dry chemical powder.
<i>Unsuitable</i>	no data

### 2. Special Hazards arising from the substance or mixture

In combustion toxic fumes may form.

### 3. Advice for Fire Fighters

Wear self-contained breathing apparatus.  
Wear protective clothing to prevent contact with skin and eyes.

## 6. Accidental Release Measures

### 1. Personal Precautions

Evacuate the area immediately.  
Do not attempt to take action without suitable protective clothing – see section 8 of SDS.

### 2. Environmental Precautions

Do not discharge into drains or rivers.  
Contain the spillage using bunding.  
Alert the neighbourhood to the presence of fumes or gas.

### 3. Methods & Materials

Mix with sand or vermiculite.  
Transfer to a closable, labelled salvage container for disposal by an appropriate method.

### 4. Preventing the occurrence of secondary hazards.

No Special Measures Required

## 7. Handling and Storage

### 1. Personal Precautions

*Safe Handling*                      Ensure there is sufficient ventilation of the area.  
P264: Wash hands thoroughly after handling.  
P270: Do not eat, drink or smoke when using this product.

*Protection against  
explosions and fires*              normal measures for preventive fire protection

### 2. Conditions for safe storage, including any incompatibilities

*Managing Storage Risks*        Store in cool, well ventilated area.  
Keep container tightly closed.

*Storage Controls*                No special requirements

*Maintaining Integrity*         Store away from oxidising agents  
Keep in tightly closed container in cool area away from direct sunlight or heat sources.

*Other advice*                      P403 + P233: Store in a well-ventilated place. Keep container tightly closed.  
no further information available

### 3. Specific End Uses

The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.

## 8. Exposure Controls/Personal Protection

### 1. Control Parameters

No Data Available

## 2. Exposure Controls

<i>General protective and hygiene measures</i>	P280: Wear protective gloves/protective clothing/eye protection/face protection. Wash hands during breaks and at the end of handling the material Immediately remove any contaminated clothing
<i>Engineering measures</i>	P271: Use only outdoors or in a well-ventilated area. Ensure there is sufficient ventilation of the area.
<i>Eye / Face Protection</i>	Safety Glasses with side-shields.
<i>Hand protection</i>	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 EU Directive 89/686/EEC 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 CE 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.
<i>Respiratory protection</i>	P260: Do not breathe dust/fume/gas/mist/vapours/spray. P284: Wear respiratory protection. Self-contained breathing apparatus must be available in case of emergency.
<i>Skin protection</i>	Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practice. Wash and dry hands. Protective clothing.
<i>Other personal protection advice</i>	no data

## 9. Physical and Chemical Properties

### 1. Physical and Chemical Properties

Appearance	Clear colourless to pale yellow liquid
Odour	No Data Available
Odour threshold	No Data Available
PH	No Data Available
Melting point / Freezing point	3°C
Initial boiling point and boiling range	189°C
Flash point	85°C
Evaporation rate	No Data Available
Flammability(solid,gas)	No Data Available
Upper/lower flammability or explosive limits	No Data Available
Vapour pressure	40Pa/20°C
Vapour density	5.56
Relative density	1.30
Solubility(ies):	Ether. Alcohol
Partition coefficient: n-octanol/water	No Data Available

Auto-ignition temperature	No Data Available
Decomposition temperature	No Data Available
Viscosity	No Data Available
Explosive properties	No Data Available
Oxidising properties	No Data Available

## 2. Other Information

No additional information available

## 10. Stability and Reactivity

### 1. Reactivity

Combustible liquid

### 2. Stability

Stable under normal conditions.

### 3. Possibility of Hazardous Reactions

Combustible liquid

### 4. Conditions to Avoid

no specific conditions to avoid

### 5. Incompatible Materials

Oxidising agents.

### 6. Hazardous Decomposition Products

In combustion emits toxic fumes.  
 In combustion emits toxic fumes of carbon dioxide / carbon monoxide.  
 In combustion emits toxic fumes of nitrogen oxides.  
 In combustion emits toxic fumes of hydrogen fluoride.

## 11. Toxicology information

### 1. Information

<i>Acute Toxicity</i>	Oral LD50 (Rat) 480mg/kg Intraperitoneal LD50 (Mouse) 50mg/kg Skin LDLo (Rabbit) 1500mg/kg
<i>Skin corrosion/irritation</i>	irritant for skin and mucous membranes
<i>Serious eye Damage/irritation</i>	irritant effect
<i>Respiratory or skin sensitisation</i>	No sensitizing effect known
<i>Germ Cell mutagenicity</i>	not known
<i>Carcinogenicity</i>	not known
<i>Reproductive toxicity</i>	not known
<i>STOT-single exposure</i>	not known
<i>STOT-repeated exposure</i>	not known
<i>Aspiration hazard</i>	not known

### 2. Additional

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.  
 No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH

## 12. Ecological Information

### 1. Toxicity

not known

## 2. Persistence and degradability

not known

## 3. Bio-Accumulative Potential

not known

## 4. Mobility and Soil

not known

## 5. Results of PBT & vPvB assessment

not known

## 6. Other adverse effects

Do not allow product to reach ground water, water bodies or sewage system, even in small quantities.  
Class 2 - Water polluting substance.

## 13. Disposal Considerations

### 1. Waste Treatment Methods

*Disposal Operations* Consult state, local or national regulations for proper disposal.

*Disposal of Packaging* Disposal must be made according to official regulations.

## 14. Transport Information

### Air (ICAO)

1. **UN Number:** 2948
2. **Shipping Name:** 3-Trifluoromethylaniline
3. **Transport hazard class(es):** : 6.1      **Sub Class :**



4. **Packing group:** II
5. **Environmental hazards:**
6. **Special Precautions for user:**
7. **Transport in bulk:**

### Road (ADR)

1. **UN Number:** 2948
2. **Shipping Name:** 3-TRIFLUOROMETHYL-ANILINE
3. **Transport hazard class(es):** : 6.1      **Sub Class :**



4. **Packing group:** II
5. **Environmental hazards:**
6. **Special Precautions for user:**
7. **Transport in bulk:**

### Sea (IMDG)

1. **UN Number:** 2948
2. **Shipping Name:** 3-Trifluoromethylaniline
3. **Transport hazard class(es):** : 6.1      **Sub Class :**



4. **Packing group:** II  
 5. **Environmental hazards:**  
 6. **Special Precautions for user:**  
 7. **Transport in bulk:** IBCINS: IBC02

UNTANKINS: T7  
TANKPROV: TP2

## 15. Safety, health, environmental and national regulations

### 1. Safety, health, environmental and national regulations:

product is not subject to any additional regulations or provisions

### 2. Safety Assessment

No Chemical Safety Assessment

## 16. Other Information

### 1. Other Information:

ADR: Accord Europeen sur le transport des marchandises Dangereuses par Route(European Agreement concerning the International Carriage of Dangerous Goods by road)  
 RID:Reglement International concernant le transport des marchandises dangereuses par chemin de fer (Regulations concerning the International transport of Dangerous Goods by Rail)  
 IMDG: International Maritime Code for Dangerous Goods  
 IATA: International Air Transport Association  
 IATA-DGR: Dangerous Goods Regulations by the International Air Transport Association  
 ICAO:International Civil Aviation Organization  
 ICAO-TI: Technical Instructions by the ICAO  
 GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
 CAS:Chemical Abstracts Service

### 2. Associated risk phrases according to european directive 67/548/EEC

R20/21/22	Harmful by inhalation, in contact with skin and if swallowed.
R20/22	Harmful by inhalation and if swallowed.
R21/22	Harmful in contact with skin and if swallowed.
R22	Harmful if swallowed.
R23	Toxic by inhalation.
R23/24	Toxic by inhalation and in contact with skin.
R23/24/25	Toxic by inhalation, in contact with skin and if swallowed.
R23/25	Toxic by inhalation and if swallowed.
R26	Very toxic by inhalation.
R26/27	Very toxic by inhalation and in contact with skin.
R26/27/28	Very toxic by inhalation, in contact with skin and if swallowed.
R26/28	Very toxic by inhalation and if swallowed.
R33	Danger of cumulative effects.
R36	Irritating to eyes.
R36/37	Irritating to eyes and respiratory system.
R36/37/38	Irritating to eyes, respiratory system and skin.
R36/38	Irritating to eyes and skin.
R37/38	Irritating to respiratory system and skin.
R38	Irritating to skin.
R48/20	Harmful: danger of serious damage to health by prolonged exposure through inhalation.
R48/20/21	Harmful: danger of serious damage to health by prolonged exposure through inhalation and in contact with skin.
R48/20/21/22	Harmful: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed.
R48/20/22	Harmful: danger of serious damage to health by prolonged exposure through inhalation and if swallowed.
R48/21	Harmful: danger of serious damage to health by prolonged exposure in contact with skin.
R48/21/22	Harmful: danger of serious damage to health by prolonged exposure in contact with skin and if swallowed.
R48/22	Harmful: danger of serious damage to health by prolonged exposure if swallowed.
R68/20/21/22	Harmful: possible risk of irreversible effects through inhalation, in contact with skin and if swallowed.
R68/20/22	Harmful: possible risk of irreversible effects through inhalation and if swallowed.

R68/21/22

Harmful: possible risk of irreversible effects in contact with skin and if swallowed.



### 3. Disclaimer

The product listed is for research and development purposes only and not for human or animal use. As such, in most cases, the toxicological, ecological and physicochemical properties have not been fully determined and the product should be treated with respect and always handled under suitable conditions by appropriately qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, to ensure proper use and protect the health and safety of employees. This information is furnished without warranty and any use of the product not in conformance with this material safety data sheet, or in combination with any other product or process, is the responsibility of the user.