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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : 4-Chlorobenzotrifluoride

Product Number : C26402

Brand : Aldrich

CAS-No. : 98-56-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Skin sensitisation (Category 1), H317

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Warning

Hazard statement(s)

H226

Flammable liquid and vapour.

H317

May cause an allergic skin reaction.

H411

Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use only non-sparking tools.

P243

Take precautionary measures against static discharge.

P261

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

P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms	:	1-Chloro-4-(trifluoromethyl)benzene 4-Chloro- $\alpha,\alpha,\alpha$ -trifluorotoluene
Formula	:	C <sub>7</sub> H <sub>4</sub> ClF <sub>3</sub>
Molecular weight	:	180.55 g/mol
CAS-No.	:	98-56-6
EC-No.	:	202-681-1

#### Hazardous components

Component	Classification	Concentration
<b>4-Chloro-<math>\alpha,\alpha,\alpha</math>-trifluorotoluene</b>		
	Flam. Liq. 3; Skin Sens. 1; Aquatic Acute 2; Aquatic Chronic 2; H226, H317, H411	90 - 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### 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. 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.

### 4.2 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

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

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 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.

### 6.3 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).

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour 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.

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

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.

### 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### 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.

**Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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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**9. PHYSICAL AND CHEMICAL PROPERTIES****9.1 Information on basic physical and chemical properties**

- |   |  |
|---|--|
| a) Appearance                                   | Form: clear, viscous liquid<br>Colour: colourless                                      |
| b) Odour  | No data available  |
| c) Odour Threshold                              | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | Melting point/range: -36 °C (-33 °F) - lit.  |
| f) Initial boiling point and boiling range      | 136 - 138 °C (277 - 280 °F) - lit.   |
| g) Flash point                                  | 43 °C (109 °F) - closed cup  |
| h) Evaporation rate                             | No data available  |
| i) Flammability (solid, gas)                    | No data available  |
| j) Upper/lower flammability or explosive limits | No data available  |
| k) Vapour pressure                              | 0.0002 hPa (0.0002 mmHg) at 25 °C (77 °F) - OECD Test Guideline 104                    |
| l) Vapour density                               | No data available  |
| m) Relative density                             | 1.353 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.  |
| n) Water solubility                             | 0.0338 g/l at 20 °C (68 °F) - slightly soluble   |
| o) Partition coefficient: n-octanol/water       | log Pow: 3.7 at 25 °C (77 °F) -  |
| p) Auto-ignition temperature                    | 600 °C (1,112 °F) at 998 hPa (749 mmHg)  |
| q) Decomposition temperature                    | No data available  |
| r) Viscosity                                    | 0.76 mm <sup>2</sup> /s at 20 °C (68 °F) - 0.58 mm <sup>2</sup> /s at 40 °C (104 °F) - |
| s) Explosive properties                         | Not explosive  |
| t) Oxidizing properties                         | No data available  |

**9.2 Other safety information**

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong bases, Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas, Hydrogen fluoride

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 13,000 mg/kg

LD50 Oral - Rat - 5,546 mg/kg

LC50 Inhalation - Rat - 4 h - > 32.03 mg/l

LD50 Dermal - Rabbit - > 3,300 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

#### Respiratory or skin sensitisation

in vivo assay - Mouse

May cause sensitisation by skin contact.  
(OECD Test Guideline 429)

#### Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: Not mutagenic in Ames Test

Chromosome aberration test in vitro

Chinese hamster ovary cells

Result: negative

#### Carcinogenicity

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

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

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

**Additional Information**

RTECS: XS9145000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Danio rerio (zebra fish) - 3 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 2 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	NOEC - Pseudokirchneriella subcapitata (green algae) - 0.41 mg/l - 72 h (OECD Test Guideline 201)

### 12.2 Persistence and degradability

Biodegradability	Result: - According to the results of tests of biodegradability this product is not readily biodegradable. (OECD Test Guideline 301D)
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### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life with long lasting effects.

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 2234      Class: 3      Packing group: III  
Proper shipping name: Chlorobenzotrifluorides  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2234      Class: 3      Packing group: III      EMS-No: F-E, S-D  
Proper shipping name: CHLOROBENZOTRIFLUORIDES

#### IATA

UN number: 2234      Class: 3      Packing group: III  
Proper shipping name: Chlorobenzotrifluorides

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### 15. REGULATORY INFORMATION

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

#### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
4-Chloro- $\alpha,\alpha,\alpha$ -trifluorotoluene	98-56-6	

#### New Jersey Right To Know Components

	CAS-No.	Revision Date
4-Chloro- $\alpha,\alpha,\alpha$ -trifluorotoluene	98-56-6	

#### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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### 16. OTHER INFORMATION

#### Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H317	May cause an allergic skin reaction.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
Skin Sens.	Skin sensitisation

#### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	2
Physical Hazard	0

#### NFPA Rating

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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