

## SAFETY DATA SHEET

Creation Date 23-Mar-2012

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Revision Number 6

### 1. Identification

**Product Name** 4-Chlorobenzotrifluoride

**Cat No. :** AC108730000; AC108730010; AC108730250; AC108732500

**CAS No** 98-56-6  
**Synonyms** 4-Chloro-alpha,alpha,alpha-trifluorotoluene; PCBTF

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

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

##### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

**Emergency Telephone Number** For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

### 2. Hazard(s) identification

#### Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids  
Skin Sensitization

Category 3  
Category 1B

#### Label Elements

**Signal Word**  
Warning

**Hazard Statements**  
Flammable liquid and vapor  
May cause an allergic skin reaction

**Precautionary Statements****Prevention**

Avoid breathing dust/fume/gas/mist/vapors/spray  
Contaminated work clothing should not be allowed out of the workplace  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
Keep container tightly closed  
Ground/bond container and receiving equipment  
Use explosion-proof electrical/ventilating/lighting equipment  
Use only non-sparking tools  
Take precautionary measures against static discharge  
Wear protective gloves/protective clothing/eye protection/face protection

**Skin**

If skin irritation or rash occurs: Get medical advice/attention  
Wash contaminated clothing before reuse  
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**Storage**

Store in a well-ventilated place. Keep cool

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Toxic to aquatic life with long lasting effects

### 3. Composition/Information on Ingredients

Component	CAS No	Weight %
p-Chloro-a,a,a-trifluorotoluene	98-56-6	>95

### 4. First-aid measures

**General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water.

**Most important symptoms and effects**

None reasonably foreseeable. May cause allergic skin reaction. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle

**Notes to Physician** pain or flushing  
Treat symptomatically

## 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray. Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	43 °C / 109.4 °F
<b>Method -</b>	CC (closed cup)
<b>Autoignition Temperature</b>	650 °C / 1202 °F
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

### Specific Hazards Arising from the Chemical

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

### Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Gaseous hydrogen fluoride (HF). Hydrogen chloride gas.

### Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

### NFPA

**Health**  
2

**Flammability**  
2

**Instability**  
0

**Physical hazards**  
N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	Do not flush into surface water or sanitary sewer system.
<b>Methods for Containment and Clean Up</b>	Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 7. Handling and storage

<b>Handling</b>	Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.
<b>Storage.</b>	Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place. Incompatible Materials. Strong oxidizing agents.

## 8. Exposure controls / personal protection

### Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
p-Chloro-a,a,a-trifluorotoluene	TWA: 2.5 mg/m <sup>3</sup>	(Vacated) TWA: 2.5 mg/m <sup>3</sup>	IDLH: 250 mg/m <sup>3</sup>	TWA: 2.5 mg/m <sup>3</sup>

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment.

**Personal Protective Equipment****Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin and body protection**

Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection**

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	Fishy
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-36 °C / -32.8 °F
Boiling Point/Range	136 - 138 °C / 276.8 - 280.4 °F @ 760 mmHg
Flash Point	43 °C / 109.4 °F
Method -	CC (closed cup)
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	38.6 mbar @ 50 °C
Vapor Density	6.23
Specific Gravity	1.350
Solubility	0.0338 g/L @ 20 °C
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	650 °C / 1202 °F
Decomposition Temperature	No information available
Viscosity	0.67 cP at 38 °C
Molecular Formula	C7 H4 Cl F3
Molecular Weight	180.56

## 10. Stability and reactivity

**Reactive Hazard**

None known, based on information available

<b>Stability</b>	Stable under normal conditions.
<b>Conditions to Avoid</b>	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Strong oxidizing agents
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Gaseous hydrogen fluoride (HF), Hydrogen chloride gas
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

### Acute Toxicity

#### Product Information

##### Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
p-Chloro-a,a,a-trifluorotoluene	LD50 = 5546 mg/kg ( Rat )	LD50 > 3300 mg/kg ( Rabbit )	LC50 = 32.03 mg/L ( Rat ) 4 h

**Toxicologically Synergistic Products** No information available

### Delayed and immediate effects as well as chronic effects from short and long-term exposure

<b>Irritation</b>	Irritating to eyes, respiratory system and skin
<b>Sensitization</b>	May cause an allergic skin reaction
<b>Carcinogenicity</b>	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
p-Chloro-a,a,a-trifluorotoluene	98-56-6	Group 2B	Not listed	Not listed	X	Not listed

<b>Mutagenic Effects</b>	No information available
<b>Reproductive Effects</b>	No information available.
<b>Developmental Effects</b>	No information available.
<b>Teratogenicity</b>	No information available.
<b>STOT - single exposure</b>	None known
<b>STOT - repeated exposure</b>	None known
<b>Aspiration hazard</b>	No information available
<b>Symptoms / effects, both acute and delayed</b>	Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting; Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting; Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing
<b>Endocrine Disruptor Information</b>	No information available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

The product contains following substances which are hazardous for the environment. Toxic to aquatic organisms, may cause

long-term adverse effects in the aquatic environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
p-Chloro-a,a,a-trifluorotoluene	Not listed	LC50 = 3 mg/L, 96h semi-static (Danio rerio) LC50 = 11.5 - 15.8 mg/L, 48h static (Lepomis macrochirus)	EC50 = 11.1 mg/L 5 min EC50 = 13.4 mg/L 15 min EC50 = 14.3 mg/L 30 min	EC50 = 2 mg/L, 48 h semi-static (Daphnia magna)

**Persistence and Degradability** Persistence is unlikely

**Bioaccumulation/ Accumulation** Not likely to bioaccumulate.

**Mobility** . Will likely be mobile in the environment due to its water solubility.

Component	log Pow
p-Chloro-a,a,a-trifluorotoluene	3.7

### 13. Disposal considerations

**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

### 14. Transport information

#### DOT

UN-No UN2234  
 Proper Shipping Name CHLOROBENZOTRIFLUORIDES  
 Hazard Class 3  
 Packing Group III

#### TDG

UN-No UN2234  
 Proper Shipping Name CHLOROBENZOTRIFLUORIDES  
 Hazard Class 3  
 Packing Group III

#### IATA

UN-No UN2234  
 Proper Shipping Name CHLOROBENZOTRIFLUORIDES  
 Hazard Class 3  
 Packing Group III

#### IMDG/IMO

UN-No UN2234  
 Proper Shipping Name CHLOROBENZOTRIFLUORIDES  
 Hazard Class 3  
 Packing Group III

### 15. Regulatory information

#### United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
p-Chloro-a,a,a-trifluorotoluene	98-56-6	X	ACTIVE	-

#### Legend:

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

U - Not Listed

T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.

**TSCA 12(b)** - Notices of Export

Component	CAS No	TSCA 12(b) - Notices of Export
p-Chloro-a,a,a-trifluorotoluene	98-56-6	Section 4

**International Inventories**

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
p-Chloro-a,a,a-trifluorotoluene	98-56-6	X	-	202-681-1	X	X	X	X	X	KE-05928

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**U.S. Federal Regulations****SARA 313**

**SARA 311/312 Hazard Categories** See section 2 for more information

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA - Occupational Safety and Health Administration** Not applicable

**CERCLA** Not applicable

**California Proposition 65** This product contains the following Proposition 65 chemicals.

Component	CAS No	California Prop. 65	Prop 65 NSRL	Category
p-Chloro-a,a,a-trifluorotoluene	98-56-6	Carcinogen	23 µg/day	Carcinogen

**U.S. State Right-to-Know Regulations**

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
p-Chloro-a,a,a-trifluorotoluene	-	X	-	-	X

**U.S. Department of Transportation**

Reportable Quantity (RQ): N  
 DOT Marine Pollutant N  
 DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**Authorisation/Restrictions according to EU REACH****Safety, health and environmental regulations/legislation specific for the substance or mixture**

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)

p-Chloro-a,a,a-trifluorotoluene	98-56-6	Listed	Not applicable	Not applicable	Not applicable
Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
p-Chloro-a,a,a-trifluorotoluene	98-56-6	Not applicable	Not applicable	Not applicable	Annex I - Y45

## 16. Other information

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### Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of SDS**