SAFETY DATA SHEET

Creation Date 23-Mar-2012 **Revision Date** 18-Dec-2025 **Revision Number** 7

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

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: 001-800-227-6701 / **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 according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 3
Skin Sensitization	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, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep container tightly closed
Ground and bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Wear protective gloves/protective clothing/eye protection/face protection
Take action to prevent static discharges
Use non-sparking tools
Skin
If skin irritation or rash occurs: Get medical advice/attention
Take off contaminated clothing and wash before reuse
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
Fire
In case of fire: Use CO2, dry chemical, or foam to extinguish
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

Hazards classified under paragraph (d)(1)(ii) of 1910.1200
No information available

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 pain or flushing

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO_2). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Unsuitable Extinguishing Media No information available

Flash Point 43 °C / 109.4 °F

Method - CC (closed cup)

Autoignition Temperature 650 °C / 1202 °F

Explosion Limits

Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	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_2). 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	Flammability	Instability	Physical hazards
2	2	0	N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Up 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

Handling 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.

Storage. 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	Mexico OEL (TWA)
p-Chloro-a,a,a-trifluorotoluene	TWA: 2.5 mg/m³	(Vacated) TWA: 2.5 mg/m³	IDLH: 250 mg/m³	TWA: 2.5 mg/m³

Legend

ACGIH - American Conference of Governmental Industrial Hygienists
OSHA - Occupational Safety and Health Administration
NIOSH: 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.

Recommended Filter type: Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State	Liquid		
Color	Colorless		
Odor	Fishy		
Odor Threshold	No information available		
Property	**Values**	**Remarks**	**• Method**
Melting Point/Range	-36 °C / -32.8 °F		
Softening Point	No data available		
Boiling Point/Range	136 - 138 °C / 276.8 - 280.4 °F	@ 760 mmHg	
Flash Point	43 °C / 109.4 °F	**Method -** CC (closed cup)	
Flammability (liquid)	Flammable	On basis of test data	
Flammability (solid,gas)	Not applicable	Liquid	
Explosion Limits	No data available		

Autoignition Temperature	650 °C / 1202 °F
Decomposition Temperature	No data available
pH	No information available
Viscosity	0.67 cP at 38 °C
Water Solubility	33.8 mg/L @ 20°C
Solubility in other solvents	No information available

Partition Coefficient (n-octanol/water)

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

Vapor Pressure	38.6 mbar @ 50 °C	
Density / Specific Gravity	1.350	
Bulk Density	Not applicable	Liquid
Vapor Density	6.23	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

Other Information

Molecular Formula	C7 H4 Cl F3
Molecular Weight	180.56
Explosive Properties	explosive air/vapour mixtures possible

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2), Gaseous hydrogen fluoride (HF), Hydrogen chloride gas

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation May produce an allergic reaction.
Ingestion May cause allergic reaction. May be harmful if swallowed.
Eyes Avoid contact with eyes. Sensitization.
Skin Avoid contact with skin. Repeated or prolonged skin contact may cause allergic reactions with susceptible persons.

Toxicology data for the components

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

(b) skin corrosion/irritation; Based on available data, the classification criteria are not met
Test method Patch Test
Test species rabbit
Observational endpoint No skin irritation

(c) serious eye damage/irritation; Based on available data, the classification criteria are not met
Test species rabbit
Observation end point fully reversible

(d) respiratory or skin sensitization;

Respiratory No data available
Skin Sub-category 1B

Component	Test method	Test species	Study result
p-Chloro-a,a,a-trifluorotoluene 98-56-6 (>95)	Local Lymph Node Assay	mouse	Sensitization

May cause an allergic skin reaction

(e) germ cell mutagenicity; Based on available data, the classification criteria are not met

Component	Test method	Test species	Study result
p-Chloro-a,a,a-trifluorotoluene 98-56-6 (>95)	in vivo	Mammalian	negative

(f) carcinogenicity;

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-trifluoro toluene	98-56-6	Group 2B	Not listed	Not listed	X	Not listed

(g) reproductive toxicity; Based on available data, the classification criteria are not met

Component	Test method	Test species / Duration	Study result
p-Chloro-a,a,a-trifluorotoluene 98-56-6 (>95)	OECD Test Guideline 415	Rat	negative

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; Based on available data, the classification criteria are not met

Test method OECD Test Guideline 413
Test species / Duration Rat
Study result NOAEC = 51 mg/m^3
Route of exposure Oral
Target Organs Liver, Digestive System, Kidney.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects,both acute and delayed 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.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

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
'-' - Not Listed
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export

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

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

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 Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
p-Chloro-a,a,a-trifluorotoluene	98-56-6	-	-	-

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

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?
See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
p-Chloro-a,a,a-trifluorotoluene (CAS #: 98-56-6)	-	-	Listed	Listed	Listed

PFAS Legend
Listed = Meets the PFAS definition of the named authority

Other International Regulations

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