

ALFAAA15154

4-Chlorobenzotrifluoride

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: 4-氯三氟甲苯
Product Description: 4-Chlorobenzotrifluoride

Cat No. : A15154
Synonyms 4-Chloro-alpha,alpha,alpha-trifluorotoluene; PCBTF
CAS No 98-56-6
Molecular Formula C7 H4 Cl F3

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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United Kingdom
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CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Colorless

Odor
Fishy

Emergency Overview

May cause an allergic skin reaction. Flammable liquid and vapor. Toxic to aquatic life with long lasting effects.

Classification of the substance or mixture

Flammable liquids.	Category 3
Skin Sensitization	Category 1B
Acute aquatic toxicity	Category 2
Chronic aquatic toxicity	Category 2

Label Elements



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Signal Word

Warning

Hazard Statements

H226 - Flammable liquid and vapor

H411 - Toxic to aquatic life with long lasting effects

H317 - May cause an allergic skin reaction

Precautionary Statements

Prevention

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P233 - Keep container tightly closed

P240 - Ground and bond container and receiving equipment

P241 - Use explosion-proof electrical/ ventilating/ lighting equipment

P242 - Use non-sparking tools

P243 - Take action to prevent static discharges

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P272 - Contaminated work clothing should not be allowed out of the workplace

P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

P333 + P313 - If skin irritation or rash occurs: Get medical advice/attention

P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P235 - Store in a well-ventilated place. Keep cool

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Vapors may cause flash fire or explosion. Flammable liquid.

Health Hazards

May cause an allergic skin reaction.

Environmental hazards

Toxic to aquatic life with long lasting effects. . Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

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

SECTION 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.

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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

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically. Symptoms may be delayed.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

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.

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.

SECTION 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.

Refer to protective measures listed in Sections 8 and 13.

SECTION 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.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Component	China	Taiwan	Thailand	Hong Kong
p-Chloro-a,a,a-trifluorotoluene	-	TWA: 2.5 mg/m ³	TWA: 2.5 mg/m ³	-

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
p-Chloro-a,a,a-trifluorotoluene	TWA: 2.5 mg/m ³	(Vacated) TWA: 2.5 mg/m ³	IDLH: 250 mg/m ³	-	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

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. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Viton (R)	See manufacturers recommendations	-	EN 374	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Long sleeved clothing

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 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

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure

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limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

Prevent product from entering drains. Do not allow material to contaminate ground water system.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Colorless	
Physical State	Liquid	
Odor	Fishy	
Odor Threshold	No data available	
pH	No information available	
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)
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	38.6 mbar @ 50 °C	
Vapor Density	6.23	(Air = 1.0)
Specific Gravity / Density	1.350	
Bulk Density	Not applicable	Liquid
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	
Autoignition Temperature	650 °C / 1202 °F	
Decomposition Temperature	No data available	
Viscosity	0.67 cP at 38 °C	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C7 H4 Cl F3	
Molecular Weight	180.56	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
Materials to avoid	Strong oxidizing agents.
Hazardous Decomposition Products	Carbon monoxide (CO). Carbon dioxide (CO ₂). Gaseous hydrogen fluoride (HF). Hydrogen chloride gas.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

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

(b) skin corrosion/irritation;

Test method

Based on available data, the classification criteria are not met

Test species

Patch Test

Observational endpoint

rabbit

No skin irritation

(c) serious eye damage/irritation;

Test species

Based on available data, the classification criteria are not met

Observation end point

rabbit

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;

No data available

There are no known carcinogenic chemicals in this product

Component	EU	UK	Germany	IARC
p-Chloro-a,a,a-trifluorotoluene				Group 2B

(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/m³

Route of exposure

Oral

Target Organs

Liver, Digestive System, Kidney.

(j) aspiration hazard;

No data available

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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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects	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.
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Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
p-Chloro-a,a,a-trifluorotoluene	LC50 = 3 mg/L, 96h semi-static (Danio rerio) LC50 = 11.5 - 15.8 mg/L, 48h static (Lepomis macrochirus)	EC50 = 2 mg/L, 48 h semi-static (Daphnia magna)		EC50 = 11.1 mg/L 5 min EC50 = 13.4 mg/L 15 min EC50 = 14.3 mg/L 30 min

Persistence and Degradability

Persistence	Persistence is unlikely.
Degradability	Not readily biodegradable.

Component	Degradability
p-Chloro-a,a,a-trifluorotoluene 98-56-6 (>95)	19.2 %, 28d

Degradation in sewage treatment plant	Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.
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Bioaccumulative Potential	Bioaccumulation is unlikely
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Component	log Pow	Bioconcentration factor (BCF)
p-Chloro-a,a,a-trifluorotoluene	3.7	122

Mobility in soil	The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils
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Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
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Contaminated Packaging	Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.
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Other Information	Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.
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SECTION 14. TRANSPORT INFORMATION

4-Chlorobenzotrifluoride

Road and Rail Transport

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

IATA

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

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
p-Chloro-a,a,a-trifluoro toluene	X	-	X	X	202-681-1	X	X	X	X	X	X	KE-05928

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department
Creation Date 23-Mar-2012
Revision Date 30-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.
Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.
First aid for chemical exposure, including the use of eye wash and safety showers.
Chemical incident response training.

Legend

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CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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 Safety Data Sheet