

Product Stewardship Summary

Parachlorobenzotrifluoride

General Statement

Parachlorobenzotrifluoride (PCBTF) is a volatile organic compound (VOC)-exempt solvent that serves as an alternative to traditional industrial solvents. PCBTF is a low to moderate hazard material and risk of adverse health effects associated with both occupational and consumer use of this chemical is anticipated to be low.

Chemical Identity

Name: Parachlorobenzotrifluoride

Brand Names: Not applicable

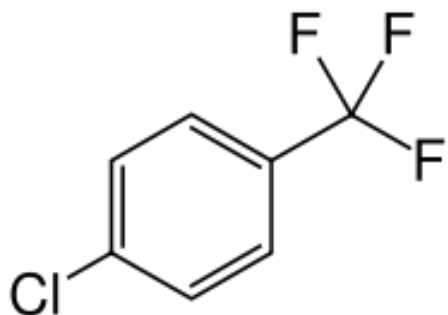
Chemical name (IUPAC): Benzene, 1-chloro-4-(trifluoromethyl)-

CAS number(s): 98-56-6

EC number: 202-681-1

Molecular formula: C₇H₄ClF₃

Structure:



Uses and Applications

PCBTF is used as an intermediate in the synthesis of dyes, pharmaceuticals, pesticides, insecticides, and herbicides, and as a solvent, mainly in paint and coating formulations.



RESPONSIBLE CARE®

© Registered trademark, Ashland or its subsidiaries, registered in various countries

™ Trademark, Ashland or its subsidiaries, registered in various countries

* Trademark owned by a third party

© 2016, Ashland



Physical/Chemical Properties

Phys/Chem Safety Assessment

Property	Value
Form	Viscous
Physical state	Liquid
Color	Colorless
Odor	Characteristic
Density	1.336 g/cm ³ @ 20°C
Melting / boiling point	-33 / 139.3 °C
Flammability	No data available
Explosive properties	Not explosive
Self-ignition temperature	600 °C
Vapor pressure	0.018 Pa @ 25°C
Mol weight	180.55 g/mol
Water solubility	84.5 mg/L @25°C
Flash point	39°C
Octanol-water partition coefficient (LogK _{ow})	3.7 @25°C

Exposure, Hazard and Safety Assessment

The following section describes possible exposure scenarios and hazards associated with parachlorobenzotrifluoride. The exposure assessment describes both the amount of and the frequency with which a chemical substance reaches a person, a population of people, or the environment. Hazard refers to the inherent properties of a substance that make it capable of causing harm to human health or the environment. The safety assessment reports the possibility of a harmful event arising from exposure to a chemical or physical agent under specific conditions. Just because a substance may possess potentially harmful properties does not mean that it automatically poses a risk. It is not possible to make that determination without understanding the exposure.

Human Health Effects

Human Exposure Assessment

Consumer: Parachlorobenzotrifluoride is used as an intermediate and as a solvent, mainly in paint and coating formulations. Consumer exposure may occur through the use of products that include PCBTF within the formulation.

Worker: In industrial settings, PCBTF is manufactured and handled in closed processes as much as possible, which ensures that worker exposure is minimized. When there is potential for exposure, during loading, unloading, sampling or during maintenance operations, exposure to PCBTF can be further minimized by the proper use of personal protective equipment.

Human Hazard Assessment:

Parachlorobenzotrifluoride is low for both acute and repeat dose toxicity. It is not irritating to the eyes or skin but may cause skin sensitization. Based on available data, it is not associated with reproductive/developmental toxicity is not mutagenic/genotoxic, and is not classified as a carcinogen.

Effect Assessment	Result
Acute Toxicity Oral / inhalation / dermal	Low toxicity following oral, dermal and inhalation exposures in experimental animals.
Irritation / corrosion Skin / eye / respiratory test	Not irritating to the skin or eyes. May cause skin sensitization.

Toxicity after repeated exposure Oral / inhalation / dermal	Does not cause significant toxicity to internal organs after repeated exposure in animal studies by oral or inhalation routes of exposure. High dose oral exposures are associated with effects on the liver and kidneys of experimental animals.
Genotoxicity / Mutagenicity	Based on available data, not considered mutagenic or genotoxic.
Carcinogenicity	Not classified as carcinogenic.
Toxicity for reproduction	Based on available data, not considered a reproductive or developmental toxicant.

Human Health Safety Assessment

Consumer: PCBTF is used as a chemical intermediate and as a solvent, mainly in paint and coating formulations. Low level inhalation and dermal exposures may occur with PCBTF if the material is present in consumer product formulations. Exposure, however, is unlikely to result in risk to human health as PCBTF has a low acute and repeat dose toxicity. Care taken to prevent dermal contact will reduce the risk of potential skin sensitization.

Worker: In industrial settings, PCBTF is manufactured and handled primarily in closed processes which limit exposure. Based on good manufacturing processes and industrial hygiene the occupational health risk associated with PCBTF is low.

Environmental Effects

Environmental Exposures

Parachlorobenzotrifluoride is moderately biodegradable and has a moderate potential for bioaccumulation. Based on its physical and chemical properties, PCBTF is expected to have low mobility in soil and will adsorb to suspended solids and sediment in the aquatic environment. Volatilization from water surfaces is expected.

Environmental Hazard Assessment

Effect Assessment	Result
Aquatic Toxicity	Considered toxic to aquatic organisms based on available data.

Fate and behavior	Result
Biodegradation	Moderately biodegradable.
Bioaccumulation potential	Moderate potential for bioaccumulation (log Kow = 3.7).
PBT / vPvB conclusion	Not considered to be either PBT or vPvB.

Environmental Safety Assessment

Care should be taken to ensure that PCBTF waste streams do not enter surface water. Based on the available data, PCBTF is considered toxic to aquatic organisms, is moderately biodegradable, and has moderate potential for bioaccumulation.

Risk Management Recommendations

Exposure to PCBTF in the workplace can be controlled by sufficient ventilation, proper handling and storage techniques, and the use of appropriate personal protective equipment as recommended in the SDS. Consumer products that contain significant levels of the substance should include necessary safety labeling and provide appropriate handling and disposal

methods.

A selection of occupational exposure limits are below.

- No known occupational exposure limits

Regulatory Agency Review

Parachlorobenzotrifluoride is on the following lists:

Australian Inventory of Chemical Substances (AICS)

China - Chemical Inventory of Existing Chemical Substances (IECSC) - CAS Numbers

Danish Environmental Protection Agency (DK-EPA) - Advisory List for Self-classification of Dangerous Substances

ECHA - List of Pre-registered Substances

Environment Canada - Domestic Substances List (DSL)

EPA - 40 CFR Part 51.100

EPA - Chemical Update System (CUS) - 2002

EPA - High Production Volume (HPV) - Chemical Hazard Data Availability

EPA - Master Testing List

EPA - Master Testing List (1996)

EPA - Office of Pollution Prevention and Toxics (OPPT) High Production Volume (HPV) Challenge Program Un-sponsored Chemicals

EPA - Office of Pollution Prevention and Toxics (OPPT) High Production Volume (HPV) Program - 1990

EPA - Regional Removal Management Levels (RML) - Chemical-specific Parameters Supporting - Density

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Diffusivity

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Henry's Law Constants

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Molecular Weight

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Organic Carbon Partition Coefficient

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Permeability Coefficient

EPA - Regional Removal Management Levels (RML) - Chemical - specific Parameters Supporting - Water Solubility

EPA - Regional Removal Management Levels (RML) - Industrial Soil Supporting (TR=1E-4, HQ=1) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Industrial Soil Supporting (TR=1E-4, HQ=3) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Residential Soil Supporting - Toxicity and Chemical-specific Information

EPA - Regional Removal Management Levels (RML) - Residential Soil Supporting (TR=1E-4, HQ=1) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Residential Soil Supporting (TR=1E-4, HQ=3) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Residential Tapwater Supporting - Toxicity and Chemical-specific Information

EPA - Regional Removal Management Levels (RML) - Residential Tapwater Supporting (TR=1E-4, HQ=1) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Residential Tapwater Supporting (TR=1E-4, HQ=3) - Carcinogenic and Noncarcinogenic SLs

EPA - Regional Removal Management Levels (RML) - Summary Table - Toxicity and Chemical-specific Information

EPA - Regional Removal Management Levels (RML) - Summary Table (TR=1E-4, HQ=1) - Screening Levels

EPA - Regional Removal Management Levels (RML) - Summary Table (TR=1E-4, HQ=3) - Screening Levels

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Density

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Diffusivity in Air and Water

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Melting Point

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Molecular Weight

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Partition Coefficients

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Tapwater Dermal Parameters

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Volatility Parameters

EPA - Regional Screening Levels (RSL) - Chemical-specific Parameters Supporting - Water Solubility

EPA - Regional Screening Levels (RSL) - Composite Worker Ambient Air - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Composite Worker Ambient Air (TR=1E-06, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Composite Worker Ambient Air (TR=1E-06, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Composite Worker Soil - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Composite Worker Soil (TR=1E-06, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Composite Worker Soil (TR=1E-06, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Ambient Air - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Resident Ambient Air (TR=1E-06, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Ambient Air (TR=1E-06, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Fish Table (TR=1E-6, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Fish Table (TR=1E-6, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Fish Table - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Resident Soil - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Resident Soil (TR=1E-06, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Soil (TR=1E-06, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Soil to Groundwater - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Resident Soil to Groundwater (TR=1E-06, HQ=0.1) - Protection of Groundwater SSLs
EPA - Regional Screening Levels (RSL) - Resident Soil to Groundwater (TR=1E-06, HQ=1) - Protection of Groundwater SSLs
EPA - Regional Screening Levels (RSL) - Resident Tapwater - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Resident Tapwater (TR=1E-06, HQ=0.1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Resident Tapwater (TR=1E-06, HQ=1) - Carcinogenic and Noncarcinogenic SLs
EPA - Regional Screening Levels (RSL) - Summary Table - Toxicity and Chemical-specific Information
EPA - Regional Screening Levels (RSL) - Summary Table (TR=1E-06, HQ=0.1) - Screening Levels
EPA - Regional Screening Levels (RSL) - Summary Table (TR=1E-06, HQ=1) - Screening Levels
EPA - Regional Screening Levels (RSL) - Summary Table (TR=1E-6, HQ=0.1) - Protection of Groundwater SSLs
EPA - Regional Screening Levels (RSL) - Summary Table (TR=1E-6, HQ=1) - Protection of Groundwater SSLs
EPA - TSCA - 8(a) - Preliminary Assessment Information Rules (PAIR)
EPA - TSCA - 8D Health and Safety Data Rule (HSDR) (a) - Specific Chemicals
EPA - TSCA - Inventory
EPA - TSCA - Test Submissions - Mega
EPA - TSCA - Test Submissions - Section 4
EPA - TSCA 4 Tests - Testing of Existing Chemicals
EPA - TSCA Section 4 Testing Results
EU - European Inventory of Existing Commercial Substances (EINECS)
International Council of Chemical Associations (ICCA) - High Production Volume (HPV) Initiative
National Cancer Institute - SMILES Notations
New Zealand - Inventory of Chemicals (NZIoC)
NTP - Nominations to the Testing Program - 2009 (Spring)
OECD - High Production Volume (HPV) Chemicals - 2004
OECD - High Production Volume (HPV) Chemicals - 200
Philippine Inventory of Chemicals and Chemical Substances (PICCS)
Regional Screening Level (RSL) Composite Worker Ambient Air (TR=1E-6, HQ=1) - Toxicity and Chemical-specific Information
Russia - Occupational Exposure Limits (OELs)

Regulatory Information / Classification and Labeling

Under the Globally Harmonized System for classification and labeling (GHS), substances are classified according to their physical, health, and environmental hazards. The hazards are communicated via specific labels and the (Extended) SDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemicals in use.

GHS Classification:

Flammable Liquids, Category 3
Skin Sensitization, Category 1

Hazard Statements:

H226: Flammable liquid and vapor.
H317: May cause allergic skin reaction

Signal Word: Warning

Precautionary Statements:

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

Hazard Pictograms:



Conclusion

Parachlorobenzotrifluoride is a useful chemical intermediate in the synthesis of dyes, pharmaceuticals, pesticides, insecticides, and herbicides, and as a solvent, mainly in paint and coating formulations. When handled responsibly, the potential for skin sensitization can be minimized, allowing consumers and workers to use materials containing PCBTF safely. Care should be taken to ensure that PCBTF waste streams do not enter surface water.

Contact Information with Company

Ashland Inc.
5200 Blazer Parkway
Dublin, Ohio 43017 <http://www.ashland.com/contact>

Date of Issue: October 17, 2016

Revision: 1

Additional Information

For more information on GHS, visit <http://www.osha.gov/dsg/hazcom/ghsguideoct05.pdf> or http://live.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html.

Ashland product stewardship summaries are located at <http://www.ashland.com/sustainability/product/product-stewardship>

Disclaimer

All statements, information and data presented herein are believed to be accurate and reliable, but are not to be taken as a guarantee, an express warranty, or an implied warranty of merchantability or fitness for a particular purpose, or representation, express or implied, for which Ashland Inc. and its subsidiaries assume legal responsibility.

REACH registration is specific to Importers/Manufacturers that place the chemical on the EU market, and is specific to registered uses. Inclusion on the list of REACH Registered Substances does not automatically imply registration by Ashland.

Inclusion on the New Zealand Inventory of Chemicals applies only to the pure substance listed. The importer of record must determine whether or not their substances are in compliance.