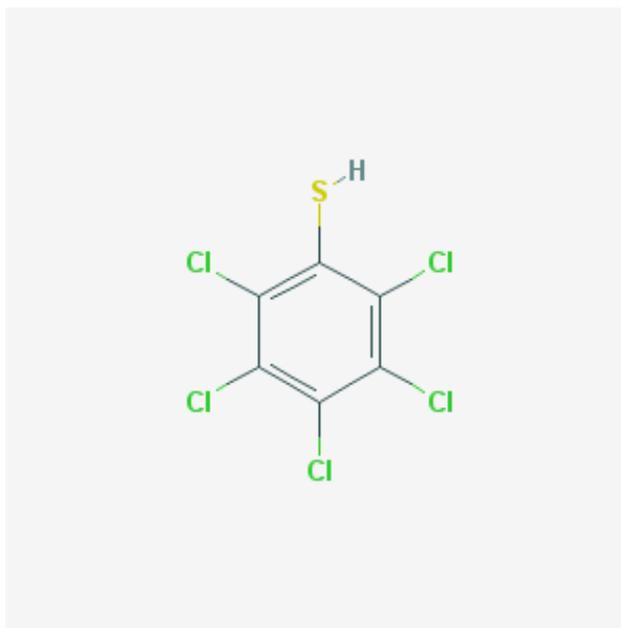


Preliminary Information on Manufacturing, Processing, Distribution, Use, and Disposal:

Pentachlorothiophenol

CASRN: 133-49-3



August 2017

Support document
for Docket EPA-HQ-OPPT-2016-0739

This document provides a preliminary public summary of available information collected by EPA's Office of Pollution Prevention and Toxics (OPPT) in the Office of Chemical Safety and Pollution Prevention (OCSPP) on the manufacturing (including importing), processing, distribution in commerce, use, and disposal of this chemical. This is based on existing data available to EPA, including information collected under the Chemical Data Reporting rule, information from other Agency databases, other U.S. Government agencies, publicly available information from states, and a review of published literature. In addition, the document includes information reported to EPA by producers and users of the chemical in the United States and in other countries.

This preliminary use information and any additional use information received in the docket by December 9, 2017, will inform efforts to identify, under section 6(h)(1)(B) of the Toxic Substances Control Act (TSCA), whether exposure to this chemical is likely, under the conditions of use, either to the environment, the general population, or to a potentially exposed or susceptible subpopulation identified by EPA. The information will also inform any risk management efforts following the exposure and use assessment under TSCA section 6(h)(1)(B).

Mention of trade names in this document does not constitute endorsement by EPA. To verify products or articles containing this chemical currently in commerce, EPA has identified several examples. Any lists are provided for informational purposes only. EPA and its employees do not endorse any of the products or companies.

This document does not contain confidential business information (CBI).

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Docket: EPA-HQ-OPPT-2016-0739

MANUFACTURING, PROCESSING, DISTRIBUTION, USE, AND DISPOSAL

1. Manufacturing (Including Importing)

No company has reported manufacture and/or import of pentachlorothiophenol (PCTP) in the U.S. above the reporting threshold of the Chemical Data Reporting (CDR) Rule for 2016¹. Only one company reported manufacture and/or import of PCTP in the U.S. in 2012². The production volume of PCTP was claimed as confidential business information (CBI).

There is no Toxics Release Inventory (TRI) data available for this chemical as it is not required to be reported under TRI³.

Manufacturing Process

PCTP is created from hexachlorobenzene (a fungicide not used in the U.S. since 1984⁴) by treatment with sodium sulfide and sulfur in methanol, or with sodium hydrogensulfide⁵. Additionally, PCTP may be created with a “reaction of hydrogen sulfide with pentachlorophenol in the presence of an acidic catalyst, eg, aluminum chloride or boron trifluoride⁶.”

¹ Manufacturers (including importers) are required to report under CDR if they meet certain production volume thresholds, generally 25,000 lb or more of a chemical substance at any single site. Reporting is triggered if the annual reporting threshold is met during any of the calendar years since the last principal reporting year. In general, the reporting threshold remains 25,000 lb per site. However, a reduced reporting threshold (2,500 lb) now applies to chemical substances subject to certain TSCA actions. <https://www.epa.gov/chemical-data-reporting/how-report-under-chemical-data-reporting>.

² https://java.epa.gov/oppt_chemical_search/; Manufacture in the context of CDR means to manufacture, produce, or import for commercial purposes. Manufacture includes the extraction, for commercial purposes, of a component chemical substance from a previously existing chemical substance or complex combination of chemical substances. (40 CFR 711.3) EPA, *TSCA Chemical Data Reporting, Fact Sheet: Importers*, (Washington DC: Office of Pollution Prevention and Toxics, 2016). https://www.epa.gov/sites/production/files/2015-12/documents/cdr_fact_sheet_importers_final_dec2015_0.pdf.

³ <https://www.epa.gov/toxics-release-inventory-tri-program/tri-listed-chemicals>

⁴ Agency for Toxic Substances and Disease Registry, *Public Health Statement: Hexachlorobenzene* (Atlanta, Georgia: Division of Toxicology and Human Health Sciences, 2015). <https://www.atsdr.cdc.gov/phs/phs.asp?id=625&tid=115>.

⁵ Roy K-M; *Thiols and Organic Sulfides*. Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2014). NY, NY: John Wiley & Sons. (Online: 2000). http://onlinelibrary.wiley.com/doi/10.1002/14356007.a26_767/full?a26_767-eo-2093#a26_767-bib-0172.

⁶ <https://pubchem.ncbi.nlm.nih.gov/compound/8620>

2. Processing

PCTP is used as a mercaptan (sulfur) cross-linking agent to make rubber more pliable in industrial uses, also called a peptizer⁷. “Natural rubber must be reduced in viscosity in order to obtain workable compounds. Many different chemical peptizers have been employed over the years for this purpose, including ... [PCTP] or its zinc salt, and dithiobisbenzanilide [135-57-9] or its zinc salt. Dithiobisbenzanilide with an activator and clay diluent is the preferred peptizing agent for natural and synthetic rubbers. The viscosity of natural rubber and synthetic polyisoprene can be reduced by mechanical shear alone, but using a peptizer makes the viscosity reduction during mixing less sensitive to variations in time and temperature, providing uniformity in viscosity from batch to batch⁸.”

3. Products and Articles

EPA identified the following types of products and articles based on a search of available sources for products containing PCTP.

According to the “Rubber Handbook” available on the website of Struktol Co of America, “STRUKTOL A95 is a 45% pentachlorothiophenol with activator on an inert filler. A95 is used for effective viscosity reduction through chemical peptization of natural rubber and synthetic rubber⁹.” Since Struktol did not submit manufacturing information to CDR in 2016, it is unclear whether this product has been discontinued, or if the manufacture/import amount has dropped below the reporting threshold.

PCTP is mentioned over 2,100 patents¹⁰ including patents held by the the following companies for the manufacture of golf balls that may include PCTP:

- Callaway Golf Co.¹¹
- Acushnet Co.¹²
- Taylor Made Golf Co.¹³
- Bridgestone Sports Co. Ltd.¹⁴

⁷ EPA, TSCA Work Plan for Chemical Assessments: 2014 Update, (Washington DC: Office of Pollution Prevention and Toxics, 2014). <https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/tsca-work-plan-chemical-assessments-2014-update>

⁸ Ohm, R. F., *Rubber Chemicals* (Online: Kirk-Othmer Encyclopedia of Chemical Technology, 2000). <http://onlinelibrary.wiley.com/doi/10.1002/0471238961.18210202150813.a01/abstract>.

⁹ Struktol, *Rubber Handbook* (Stow, Ohio: 2004). <http://www.struktol.com/pdfs/RubberHB.pdf>.

¹⁰ <https://pubchem.ncbi.nlm.nih.gov/compound/8620>

¹¹ <http://www.google.com.ar/patents/US7199192?cl=en>

¹² <https://www.google.com/patents/US20090181801?cl=en>; <http://www.google.tt/patents/US20110237352>

¹³ <https://patents.google.com/patent/US20060172823A1/en>

¹⁴ <https://patents.google.com/patent/US6679791B2/en>

4. Distribution (Includes Retailers)

General internet searches for distributors of PCTP yielded many vendors selling various quantities at different purities. Note that these are defined as distributors due to their marketing of PCTP for sale and distribution. Results of a search of distributors of PCTP are in Table 1 below. This list is provided for informational purposes only. EPA and its employees do not endorse any of the products or companies.

Table 1. Distributors of PCTP

Name	Available Quantity	Purity (%)	Reference
PCTP	100 mg	Not specified	http://www.sigmaaldrich.com/catalog/product/supelco/met12159b?lang=en&region=US&cm_sp=insite--prodRecCold_xviews--prodRecCold10-1
PCTP	25g	>95.0%(T)	http://www.tcichemicals.com/eshop/en/us/commodity/P0312/
PCTP	1g	98%	http://www.jkchemical.com/EN/products/A01371068.html
PCTP	5g	98%	http://www.jkchemical.com/EN/products/A01371068.html
PCTP	100mg	Not specified	http://en.meryer.com/en/products/detail.aspx?ProID=117134
PCTP	25g	95%	http://en.meryer.com/en/products/detail.aspx?ProID=117133
PCTP	25g	>95.0%(T)	http://www.tcichemicals.com/eshop/en/hk/catalog/list/search?searchWord=133-49-3&client=default_frontend&output=xml_no_dtd&proxystylesheet=default_frontend&sort=date%3AD%3A%3Ad1&oe=UTF-8&ie=UTF-8&ud=1&exclude_apps=1&site=en_hk&mode=0
PCTP	Up to kgs	98%(Min,HPLC)	http://www.capotchem.com/133-49-3.html
PCTP	25g	95%	https://www.abcr.de/shop/en/AB140076
PCTP	Quote provided upon request	Not specified	http://www.tractuschem.com/productshow/TRA0021029.html
PCTP	Backordered; Price not available	96%	http://www.aurumpharmatech.com/Product/ProductDetails/K_4195
PCTP	Quote provided upon request	Not specified	http://www.vitasmlab.com/index.php?option=com_search_stk&Itemid=22&stk=BBL028077&?utm_source=pubchem&utm_medium=p_search_link&utm_campaign=pubchem_search&utm_content=pubchem_slink
PCTP	Quote provided upon request	Not specified	http://www.apichemistry.com
PCTP	Quote provided upon request	Not specified	http://www.1717chem.com/

Name	Available Quantity	Purity (%)	Reference
PCTP	Quote provided upon request	Not specified	http://www.akosgmbh.de/AKosSamples/index.html
PCTP	Quote provided upon request	Not specified	http://www.debyesci.com/
PCTP	Quote provided upon request	Not specified	http://www.anpharma.net
PCTP	Quote provided upon request	Not specified	http://www.ichemical.com/chemicals/cas-133-49-3
PCTP	Quote provided upon request	Not specified	https://www.biosynth.com/en/products/chemical-intermediates/advanced-intermediates/products/Q-201540.html
PCTP	10mg	92%	https://mcule.com/MCULE-6962967512/
PCTP	Up to 25g minimum order value required	>95%	http://online.aurorafinechemicals.com/info?ID=A13.141.039
PCTP	Quote provided upon request	Not specified	https://aksci.com/item_detail.php?cat=M803
PCTP	Quote provided upon request	Not specified	http://www.anward.com/pro_result/28277/
PCTP	50g	95%	http://www.labseeker.com/goods.php?id=24282
PCTP	Quote provided upon request	Not specified	http://www.achemica.com
PCTP	Quote provided upon request	Not specified	http://www.chemtik.com
PCTP	Quote provided upon request	97%	http://www.rennotech.com/product_show.asp?id=28872
PCTP	Quote provided upon request (research only but not for commercial purposes)	Not specified	http://www.chembopharma.com
PCTP	500g	98%	http://www.ahhchemical.com/product/MT-20665.html
PCTP	100mg	Not specified	https://www.scbt.com/scbt/product/pentachlorothiophenol-133-49-3

5. Uses

Industrial Uses

Chemical peptizers are used to reduce viscosity during the production of rubber materials. “For many years the preferred peptizer was PCTP or its zinc salt. Meanwhile PCTP is banned in most parts of the world because it forms several teratogenic decomposition products. PCTP is replaced by 2,2'-dibenzamidodiphenyldisulfide (DBD) which is less toxic and reacts similarly¹⁵.”

Uniroyal, Inc., now owned by Michelin, owned a patent for producing pentachloronitrobenzene, a soil fungicide, by the reaction of PCTP with nitric acid in the presence of sulfuric acid or oleum¹⁶.

Naphthalene can be extracted from aqueous samples with PCTP -gold colloid on magnetic microparticles¹⁷.

The Swedish Chemicals Agency KEMI Commodity Guide suggests that PCTP may be found in butadiene rubber, isoprene rubber, natural rubber, and other rubber materials¹⁸. So it is possible that imported products containing these materials could contain PCTP. However, a letter to EPA from the Rubber Manufacturers Association, dated Feb. 22, 2017, indicates that its members “do not currently use ... PCTP to manufacture tires produced in the U.S. or imported into the U.S.”¹⁹.”

Commercial Uses

Commercially available PCTP is used in laboratories for research purposes. See Section 4 above.

Consumer Uses

EPA is not aware of consumer uses for PCTP.

¹⁵ Engels H-W et al; *Rubber, 9. Chemicals and Additives*. Ullmann's Encyclopedia of Industrial Chemistry 7th ed. (1999-2014) (New York, New York: John Wiley & Sons, 2014).

http://onlinelibrary.wiley.com/doi/10.1002/14356007.a23_365.pub3/pdf.

¹⁶ <https://www.google.com/patents/US4454362>

¹⁷ Mosier-Boss PA, Lieberman SH, *Surface-enhanced Raman spectroscopy substrate composed of chemically modified gold colloid particles immobilized on magnetic microparticles*, (Anal. Chem., 2005).

<https://www.ncbi.nlm.nih.gov/pubmed/15858982>.

¹⁸ <http://www.kemi.se/en/directly-to/statistics/the-commodity-guide>

¹⁹ Amick, *Hexachlorobutadiene (HCBD) and Pentachlorothio-phenol (PCTP) not currently used to make RMA member company tires manufactured in the U.S. or imported into the U.S.*, Ltr to Doug Parsons, from Rubber Manufacturers Association, Feb. 22, 2017. EPA-HQ-OPPT-2016-0739-0002

6. Disposal of Waste and Recycling/Recovery

PCTP is not regulated as hazardous waste. EPA is not aware of information regarding the recycling and recovery of PCTP, nor the disposal of PCTP as waste.

USEFUL TYPES OF INFORMATION

This document presents a summary of information currently available to EPA on this chemical. EPA is interested in obtaining information to more fully characterize the manufacturing, processing, distribution, disposal, and use of this chemical, to inform the development of the exposure and use assessment for this chemical, and to inform any subsequent risk management efforts. For example, EPA is interested in obtaining information on:

- the functional uses for this chemical;
- what types of products contain this chemical;
- which industry sectors use this chemical;
- what volume of the chemical is used;
- which uses have been discontinued or phased out;
- exposure scenarios for this chemical; and
- in which articles this chemical is found.

APPENDIX: ADDITIONAL SOURCES CONSULTED

- U.S. EPA *Chemical Inventory*
<https://www.epa.gov/tsca-inventory>
- U.S. National Library of Medicine *ChemIDplus*
<https://chem.sis.nlm.nih.gov/chemidplus/>
- U.S. EPA *SRS*
https://iaspub.epa.gov/sor_internet/registry/substreg/searchandretrieve/substancesearch/search.do
- U.S. EPA *HPV HC* (access through Chemical Data Access Tool – CDAT)
https://java.epa.gov/oppt_chemical_search/
- U.S. National Library of Medicine *Hazardous Substance Data Bank (HSBD)*
<https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- U.S. EPA *HPVIS* and *HPV HC* (access through Chemical Data Access Tool – CDAT)
https://java.epa.gov/oppt_chemical_search/
- SRC *FatePointers Search Module PHYSPROP*
<http://esc.syrres.com/fatepointer/search.asp>

- U.S. EPA *Superfund chemical data matrix* <https://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query>
- U.S. EPA *ChemView* <https://java.epa.gov/chemview>
- U.S. EPA *InertFinder* <https://iaspub.epa.gov/apex/pesticides/f?p=101:1:>
- U.S. EPA *Pesticide Chemical Search* <https://iaspub.epa.gov/apex/pesticides/f?p=CHEMICALSEARCH:1:0::NO:1::>
- U.S. EPA *Endocrine Disruptor Screening Program* <https://www.epa.gov/ingredients-used-pesticide-products/endocrine-disruptor-screening-program-tier-1-assessments>
- U.S. EPA *Hazardous Air Pollutants* <https://www.epa.gov/haps/initial-list-hazardous-air-pollutants-modifications>
- U.S. EPA *Significant New Alternatives Policy (SNAP)* <https://www.epa.gov/snap>
- U.S. EPA *Volatile Organic Compounds* <https://www.epa.gov/indoor-air-quality-iaq/technical-overview-volatile-organic-compounds#definition>
- U.S. EPA *Toxic and priority pollutants under the Clean Water Act* <https://www.epa.gov/eg/toxic-and-priority-pollutants-under-clean-water-act#toxic>
- U.S. EPA *Contaminant Candidate list under the Safe Drinking Water Act* <https://www.epa.gov/ccl/contaminant-candidate-list-3-ccl-3#chemical-list>
- U.S. EPA *IRIS Assessment* <https://cfpub.epa.gov/ncea/iris2/atoz.cfm>
- OSHA *Chemical Hazards and Toxic Substances* <https://www.osha.gov/SLTC/hazardoustoxicsubstances/index.html>
- NIOSH *Workplace Safety and Health Topics Chemicals* <http://www.cdc.gov/niosh/topics/chemical.html>
- NIOSH *Pocket Guide to Chemical Hazards* <http://www.cdc.gov/niosh/npg/npgdcas.html>
- CPSC *Chemicals* <http://www.cpsc.gov/en/Research--Statistics/Chemicals/>
- CPSC *FHSA* <https://www.cpsc.gov/Business--Manufacturing/Business-Education/Business-Guidance/FHSA-Requirements/>
- Food and Drug Administration *List of Databases* <http://www.fda.gov/ForIndustry/FDABasicsforIndustry/ucm234631.htm>
- NTP (National Toxicology Program) *Substances studied by NTP* <http://ntpsearch.niehs.nih.gov/?e=True&ContentType=Testing+Status>
- Department of Energy *Protective Action Criteria Database* <http://energy.gov/ehss/protective-action-criteria-pac-aegls-erpgs-teels-rev-29-chemicals-concern-may-2016>

- California DTSC *Toxics in Products*
<http://www.dtsc.ca.gov/PollutionPrevention/ToxicsInProducts/index.cfm>
<http://www.dtsc.ca.gov/SCP/CandidateChemicalsList.cfm>
<http://www.dtsc.ca.gov/SCP/WhatIsAPriorityProduct.cfm>
- California OEHHA *Biomonitoring*
<http://biomonitoring.ca.gov/chemicals>
- California *Permissible exposure limits for chemical contaminants*
https://www.dir.ca.gov/title8/5155table_ac1.html
- California *Hazardous substance list*
<https://www.dir.ca.gov/title8/339.html>
- California *Safe Cosmetics Program – list of chemical agents known or suspected to cause cancer or developmental or other reproductive harm.*
<http://www.cdph.ca.gov/programs/cosmetics/Pages/default.aspx>
- Maine *Chemicals of high concern* <http://www.maine.gov/dep/safechem/highconcern/>
- Michigan *Environmental Health Topics* http://www.michigan.gov/mdhhs/0,5885,7-339-71548_54783_54784_74881-13050--,00.html
- New Hampshire *Regulated Toxic Air Pollutants*
<http://des.nh.gov/organization/commissioner/legal/rules/documents/env-a1400.pdf>
- New Jersey *Right to Know Hazardous Substances*
<http://web.doh.state.nj.us/rtkhsfs/rtkhsl.aspx>
- Oregon *Priority Persistent Pollutants (in water)*
<http://www.deq.state.or.us/wq/SB737/>
- Oregon *Pollutant Profiles*
<http://www.deq.state.or.us/wq/SB737/docs/LegRpAtt420100601.pdf>
- Oregon *Reducing Toxics in Oregon*
<http://www.oregon.gov/deq/Pages/ToxicsReduction.aspx>
- Oregon *Chemicals of Concern for Children’s Health*
<http://public.health.oregon.gov/HealthyEnvironments/HealthyNeighborhoods/ToxicSubstances/Pages/childrens-chemicals-of-concern.aspx>
- Pennsylvania Department of Labor and Industry *Hazardous Substance List*
<http://www.pacode.com/secure/data/034/chapter323/chap323toc.html>
- Rhode Island *Air Resources – Air Toxics*
http://www.dem.ri.gov/pubs/regs/regs/air/air22_08.pdf
- Vermont *Chemical Disclosure Program for Children’s Products*
<http://www.healthvermont.gov/enviro/chemical/cdp.aspx>
- Washington *Chemicals of High Concern to Children*
<http://www.ecy.wa.gov/programs/hwtr/rtt/cspa/chcc.html>
- Washington *Children’s Safe Products Act*
<http://apps.leg.wa.gov/RCW/default.aspx?cite=70.240>
- Washington Department of Labor & Industries *SHARP Publications*
<http://www.lni.wa.gov/Safety/Research/Pubs/default.asp>
- Lowell Center for Sustainable Production *Chemical, Policy and Science Initiative*
<http://www.chemicalspolicy.org/chemicalspolicy.us.state.database.php>

- National Conference of State Legislatures <http://www.ncsl.org/research/environment-and-natural-resources/state-chemical-statutes.aspx>
- OECD *eChemPortal*
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- Stockholm Convention on Persistent Organic Pollutants
<http://chm.pops.int/TheConvention/ThePOPs/ListingofPOPs/tabid/2509/Default.aspx>
<http://chm.pops.int/TheConvention/ThePOPs/ChemicalsProposedforListing/tabid/2510/Default.aspx>
- WHO IPCS (UN)
<http://www.who.int/ipcs/en/>
- Other – worker protection information
<http://www.dguv.de/ifa/gestis/gestis-internationale-grenzwerte-fuer-chemische-substanzen-limit-values-for-chemical-agents/index-2.jsp>
- U.S. EPA *Chemical and Product Categories (CPCat) Database*
<https://actor.epa.gov/cpcat/faces/home.xhtml>
- U.S. National Library of Medicine *Hazardous Substance Data Bank (HSBD)*
<https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- CPSC *Chemicals*
<http://www.cpsc.gov/en/Research--Statistics/Chemicals/>
- U.S. Department of Health & Human Services *Household Products Database*
<https://hpd.nlm.nih.gov/index.htm>
- DeLima Associates *Consumer Product Information Database (CPID)*
<https://www.whatsinproducts.com/chemicals/index/1>
- Product and company websites
<https://safecosmetics.cdph.ca.gov/search/Default.aspx>
- U.S. EPA *Hazardous Waste*
<https://www.epa.gov/hw/learn-basics-hazardous-waste#regulations>
- Pollution Prevention information, including TRI
<https://www.epa.gov/p2/pollution-prevention-tools-and-calculators>
- DfE Alternatives Assessments
<https://www.epa.gov/saferchoice/design-environment-alternatives-assessments>
- Safer Chemical Ingredients List
<https://www.epa.gov/saferchoice/safer-ingredients>
- Green Chemistry awards – information regarding possible alternatives
<https://www.epa.gov/greenchemistry/presidential-green-chemistry-challenge-winners>
- Pollution Prevention – information regarding possible alternatives
<https://www.epa.gov/p2/pollution-prevention-case-studies>
<https://www.epa.gov/p2/grant-programs-pollution-prevention#sra>
- Greener products and services (e.g. some of the electronic standards include alternative assessments)
<https://www.epa.gov/greenerproducts/identify-greener-products-and-services>