Compound Information

Chemical Names: 3,3',4,4',5-Pentachlorobiphenyl

3,4,5,3',4'-Pentachlorobiphenyl

3,3',4,4',5-Pentachloro-1,1'-biphenyl

PCB 126

Chemical formula: $C_{12}H_5Cl_5$

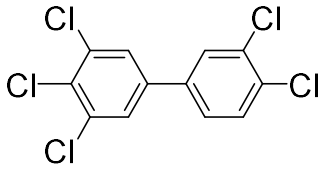
Molecular weight: 326.42

PubChem CID: 63090

InChl Key: REHONNLQRWTIFF-UHFFFAOYSA-N

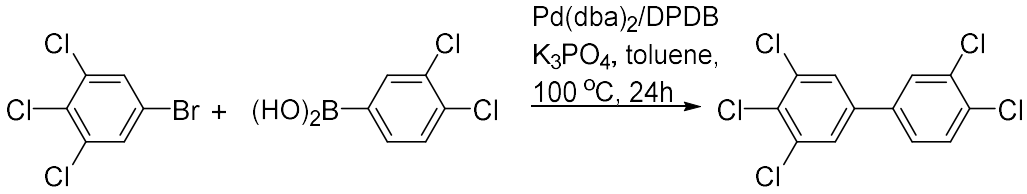
CAS number: 57465-28-8

Structure:



Synthesis: Suzuki Cross Coupling reaction between 3,4,5-trichlorobromobenzene and 3,4-dichlorophenylboronic acid under the catalysis of $Pd(dba)_2$/DPDB system (Joshi et al., 2011).

Reaction scheme:



GC-MS (*m/z*): 323.9, 254.0, 218.0, 184.0 (Gadupudi et al., 2018)

Purification: Flash column chromatography (silica-gel and hexane)

Purity: > 99% by GC-MS, detail of analysis method see reference (Li et al., 2018)

State: White solid

Melting Point: 158-160 °C

Instruments and software used to record and process raw data

Files	Instruments for raw data	Software to process raw data
^{1}HNMR raw.rar	Bruker AV500 spectrometer in the University of Iowa Central NMR Research Facility (Iowa City, IA, USA)	Spectrometer software: Vnmr Varian, Vnmr J Varian, TopSpin Bruker Other software: Mnova, NMRPipe, ACD, SpinWorks, matNMR
^{13}CNMR raw.rar	Bruker AV500 spectrometer in the University of Iowa Central NMR Research Facility (Iowa City, IA, USA)	Spectrometer software: Vnmr Varian, Vnmr J Varian, TopSpin Bruker Other software: Mnova, NMRPipe, ACD, SpinWorks, matNMR
GC-MS raw.D.rar	Mass spectra of all compounds were recorded on an Agilent 7890A gas chromatograph equipped with an Agilent 5975C Inert Mass Selective Detector (Agilent Technologies, CA, USA)	Agilent ChemStation is commonly used to process the raw data in .d format. Raw data can be converted into the desired format using ProteoWizard software.

Reference:

Gadupudi GS, Elser BA, Sandgruber FA, Li X, Gibson-Corley KN & Robertson LW (2018) PCB126 inhibits the activation of AMPK-CREB signal transduction required for energy sensing in liver. Toxicol. Sci. 163: 440-453.

Joshi SN, Vyas SM, Duffel MW, Parkin S & Lehmler HJ (2011) Synthesis of Sterically Hindered Polychlorinated Biphenyl Derivatives. Synthesis: 1045-1054.

Li X, Holland EB, Feng W, Zheng J, Dong Y, Pessah IN, Duffel MW, Robertson LW & Lehmler HJ (2018) Authentication of synthetic environmental contaminants and their (bio)transformation products in toxicology: polychlorinated biphenyls as an example. Environ Sci Pollut Res 25: 16508-16521.