Compound Information

Name:
- 4-Chloro-3',4'-dihydroxy-biphenyl
- 1,2-Dihydroxy-4'-chloro-biphenyl
- 4-(4-Chlorophenyl)benzene-1,2-diol

Chemical formula: $C_{12}H_9ClO_2$

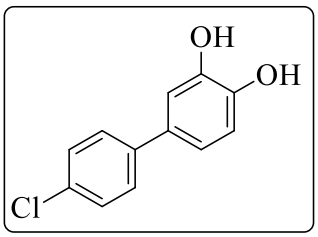
Molecular weight: 220.6520

PubChem CID: 108673 (https://pubchem.ncbi.nlm.nih.gov/compound/108673)

InChl Key: SCKSZDPELRSPES-UHFFFAOYSA-N

CAS number: 55097-84-2

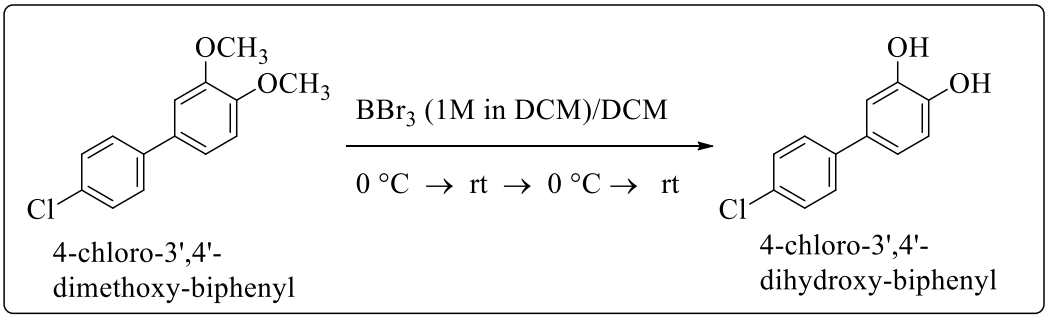
Structure:



Synthetic route: Demethylation with BBr_3

Synthesis: 4-Chloro-3',4'-dimethoxy-biphenyl undergoes demethylation with BBr_3 to provide 4-chloro-3',4'-dihydroxy-biphenyl

Reaction:



^{1}H NMR: 500 MHz, $CDCl_3$) δ = 7.44 (AA'XX' system, 2H), 7.36 (AA'XX' system, 2H), 7.08 (d, *J* = 2.0 Hz, 1H), 7.02 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 5.20 (s, 1H), 5.15 (s, 1H) ppm

^{13}C NMR	126 MHz, $CDCl_3$ δ = 143.9, 143.4, 139.2, 133.8, 133.1, 129.0, 128.1, 120.0, 116.0, 114.3 ppm
Purification:	Recrystallization (7:3; hexane/chloroform)
Color and state:	White solid
Melting point:	124-125 °C (literature melting point: 121-122 °C)

Reference:

1. McLean, M. R.; Bauer, U.; Amaro, A. R.; Robertson, L. W. (1996) Identification of catechol and hydroquinone metabolites of 4-monochlorobiphenyl. *Chem Res Toxicol* 9, 158-164

2. Wetzel, A.; Ehrhardt, V.; Heinrich, M. R. (2008) Synthesis of amino- and hydroxybiphenyls by radical chain reaction of arenediazonium salts. *Angew Chem Int Ed* **47**, 9130-9133

Instruments and software used to record and process raw data for ***4-chloro-3',4'-dihydroxy-biphenyl***

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.