Compound Information

Name:
- 4-Chloro-3-hydroxy-biphenyl
- 3-Hydroxy-4-chloro-biphenyl
- 4-Chloro-biphenyl-3-ol
- 2-Chloro-5-phenylphenol

Chemical formula: $C_{12}H_9ClO$

Molecular weight: 204.65304

PubChem CID: 519602 (https://pubchem.ncbi.nlm.nih.gov/compound/519602)

InChl Key: JLOLMJZKXRFOOE-UHFFFAOYSA-N

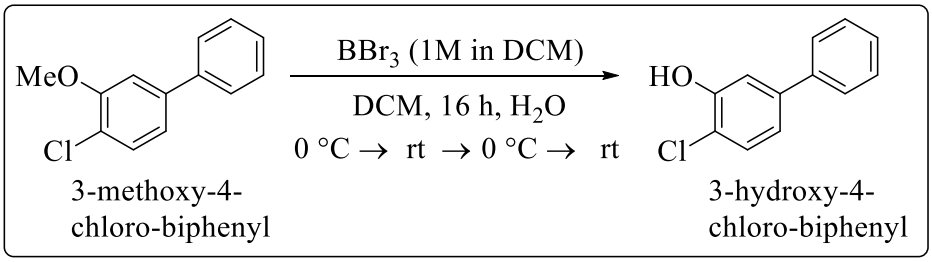
CAS number: 18773-38-1

Structure:

Synthetic route: Demethylation with BBr_3

Synthesis: 3-Methoxy-4-chlorobiphenyl undergoes demethylation with BBr_3 to provide 4-chloro-3-hydroxy-biphenyl

Reaction:



^{1}H NMR: 500 MHz, $CDCl_3$, δ 7.59 (AA'XX' system, 2H), 7.48 (m, 2H), 7.37 (AA'XX' system, 2H), 7.30 (d, *J* = 2.1 Hz, 1H), 7.15 (dd, *J* = 8.3, 2.1 Hz, 1H), 5.61 (s, 1H) ppm

^{13}C NMR:	126 MHz, $CDCl_3$ δ = 151.6, 142.0, 140.0, 129.3, 129.0, 127.9, 127.1, 120.3, 119.1, 115.0 ppm
GC-MS:	*m/z* (relative abundance %): 204.0 ($M^{\cdot+}$, 100), 139.1 (37), 115.1 (11)
Purification:	Flash column chromatography (silica-gel and hexane) and recrystallization (1:7; chloroform/hexane)
Purity:	>99% (determined based on relative peak area by GC-MS)
State:	White solid

Reference:

1. Zhai, G.; Lehmler, H.-J.; Schnoor, J. L. (2011) New hydroxylated metabolites of 4-monochlorobiphenyl in whole poplar plants. *Chem Cent J* **5:**87

2. 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**, 158-154

*Instruments and software used to record and process raw data for **4-chloro-3-hydroxy-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.