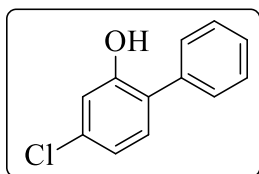


Compound Information

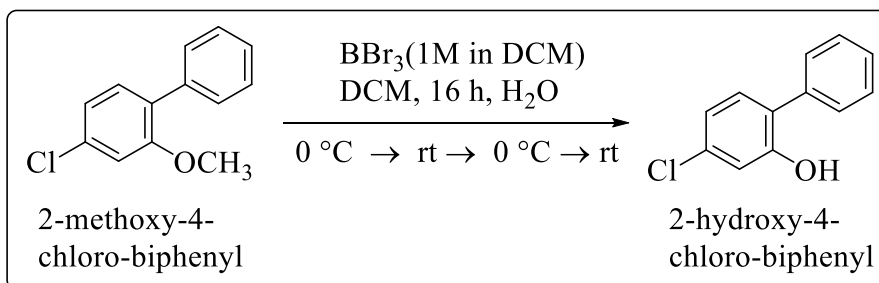
Name:	<ul style="list-style-type: none"> • 4-Chloro-2-hydroxy-biphenyl • 2-Hydroxy-4-chloro-biphenyl • 4-Chloro-biphenyl-2-ol
Chemical formula:	C ₁₂ H ₉ ClO
Molecular weight:	204.65304
PubChem CID:	13956205 (https://pubchem.ncbi.nlm.nih.gov/compound/13956205)
InChI Key:	LMUKIFZFZRTUIY-UHFFFAOYSA-N
CAS number:	91498-69-0

Structure:



Synthetic route:	Demethylation with BBr ₃
Synthesis method:	2-Methoxy-4-chloro-biphenyl undergoes demethylation with BBr ₃ to provide 2-hydroxy-4-chloro-biphenyl

Reaction:



¹ H NMR:	500 MHz, CDCl ₃ , δ = 7.53 – 7.46 (m, 2H), 7.45 – 7.40 (m, 3H), 7.16 (d, <i>J</i> = 8.1 Hz, 1H), 7.03 – 6.95 (m, 2H), 5.24 (s, 1H) ppm
¹³ C NMR:	126 MHz, CDCl ₃ , δ = 153.2, 136.1, 134.5, 131.1, 129.6, 129.1, 128.4, 126.9, 121.4, 116.3 ppm

GC-MS:	m/z (relative abundance %): 204.0 (M^+ , 100), 168.1 (36), 139.1 (33), 115.1 (21)
Purification:	Flash column chromatography (silica-gel and hexane)
R _f :	0.375 (9:1; hexane: ethyl acetate, silica-gel TLC glass plate)
Purity:	>99% (determined based on relative peak area by GC-MS)
State:	Colorless oil

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

Instruments and software used to record and process raw data for 2-hydroxy-4-chloro-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.