Compound Information

Name:
- 4-Chloro-2'-methoxy-biphenyl
- 4'-Chloro-2-methoxy-biphenyl

Chemical formula: $C_{13}H_{11}ClO$

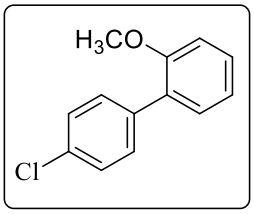
Molecular weight: 218.6800

PubChem CID: 12648515 (https://pubchem.ncbi.nlm.nih.gov/compound/12648515)

InChl Key: MBOXSXIGVXMZDU-UHFFFAOYSA-N

CAS number: 53824-23-0

Structure:



GC-MS: *m/z* (relative abundance %): 218.1 (M^{+}, 100), 203.0 (14), 168.1 (M^{+} - CH_3Cl, 100), 139.1 (37)

Purity: >99% (determined based on relative peak area by GC-MS)

State: White solid

References:

1. Li, X.; Robertson, L. W.; Lehmler, H.-J. (2009) Electron ionization mass spectral fragmentation study of sulfation derivatives of polychlorinated biphenyls. *Chem Cent J* **3**, 5

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

*Instruments and software used to record and process raw data for **4-chloro-2'-methoxy-biphenyl***

File	Instruments for raw data	Software to process raw data
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.