Compound information

IUPAC Name: 5-Bromo-3-chloro-1,2-dimethoxybenzene or 5-bromo-1-chloro-2,3-dimethoxy-benzene

Chemical formula: $C_8H_8BrClO_2$

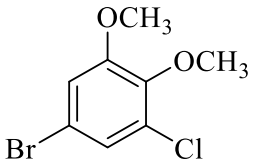
Molecular weight: 251.50

PubChem CID: 125116436

InChl Key: QFKWVYTVPILSLU-UHFFFAOYSA-N

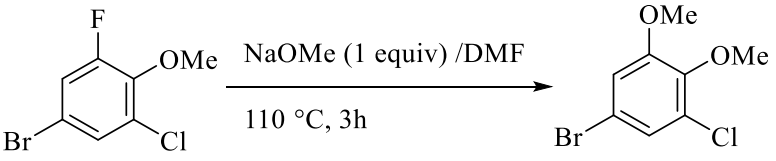
CAS number: 1881332-60-0

Structure:



Synthetic route: Nucleophilic aromatic substitution (S_NAr)

Reaction scheme:



4-bromo-2-chloro-6-fluoroanisole

5-Bromo-1-chloro-2,3-dimethoxybenzene

Keywords:

Authentication, aromatic nucleophilic substitution, precursor, superfund chemicals, methoxy compound

Funding:

ES027169, ES013661, ES005605

Table of contents for 5-bromo-3-chloro-1,2-dimethoxybenzene

SN	Name of files	Data taken instrument	Raw data processing
1.	^{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
2.	^{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
3.	GC-MS raw.D.rar	Mass spectra of all compounds were recorded on an Agilent 7890A gas chromatograph (GC) equipped with an Agilent 5975C Inert Mass Selective Detector (Agilent Technologies, CA, USA)	Agilent ChemStation is commonly used to process the raw data of .d format. Many raw data can be converted into the desired format using ProteoWizard software.