

4-Bromoguaiacol, tert-butyldimethylsilyl ether

Other names:	4-Bromoguaiacol, tbdms derivative
Inchi:	InChI=1S/C13H21BrO2Si/c1-13(2,3)17(5,6)16-11-8-7-10(14)9-12(11)15-4/h7-9H,1-6H3
InchiKey:	QMCJWKWEGJPWMG-UHFFFAOYSA-N
Formula:	C13H21BrO2Si
SMILES:	COc1cc(Br)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	317.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	4.842		Crippen Method
rinpola	1750.50		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/116-870-7/4-Bromoguaiacol-tert-butyldimethylsilyl-ether.pdf>

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