

3-Methoxythiophenol, S-(tert-butyldimethylsilyl)-

Other names:	3-Methoxythiophenol, tbdms derivative
Inchi:	InChI=1S/C13H22OSSi/c1-13(2,3)16(5,6)15-12-9-7-8-11(10-12)14-4/h7-10H,1-6H3
InchiKey:	DUABUMRLWCNOGX-UHFFFAOYSA-N
Formula:	C13H22OSSi
SMILES:	COc1cccc(S[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	254.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	4.792		Crippen Method
rinpol	1721.60		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352996&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/123-849-3/3-Methoxythiophenol-S-tert-butyldimethylsilyl.pdf>

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