

4-(Methylmercapto)phenol, tert-butyldimethylsilyl ether

Other names:	4-(Methylthio)phenol, tbdms derivative
Inchi:	InChI=1S/C13H22OSSI/c1-13(2,3)16(5,6)14-11-7-9-12(15-4)10-8-11/h7-10H,1-6H3
InchiKey:	MUPJZCSYDGGJACK-UHFFFAOYSA-N
Formula:	C13H22OSSI
SMILES:	CSc1ccc(O[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]:	254.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	4.792		Crippen Method
rinpol	1712.20		NIST Webbook
rinpol	1712.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/18-962-4/4-Methylmercapto-phenol-tert-butyldimethylsilyl-ether.pdf>

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