

1,2-Benzenedithiol, S-(tert-butyldimethylsilyl)-

Other names:	1,2-Benzenedithiol, tbdms derivative
Inchi:	InChI=1S/C12H20S2Si/c1-12(2,3)15(4,5)14-11-9-7-6-8-10(11)13/h6-9,13H,1-5H3
InchiKey:	SHUFJTURCMWMAG-UHFFFAOYSA-N
Formula:	C12H20S2Si
SMILES:	CC(C)(C)[Si](C)(C)Sc1ccccc1S
Mol. weight [g/mol]:	256.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	5.073		Crippen Method
rinpol	1788.60		NIST Webbook

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=U353066&Units=SI

Legend

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

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<https://www.chemeo.com/cid/18-186-6/1-2-Benzenedithiol-S-tert-butyldimethylsilyl.pdf>

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