

1,3-Benzenedithiol, S,S'-bis(tert-butyldimethylsilyl)-

Other names: 1,3-Benzenedithiol, 2tbds derivative
Inchi: InChI=1S/C18H34S2Si2/c1-17(2,3)21(7,8)19-15-12-11-13-16(14-15)20-22(9,10)18(4,5)6
InchiKey: LOVVMWDERRMTMA-UHFFFAOYSA-N
Formula: C18H34S2Si2
SMILES: CC(C)(C)[Si](C)(C)Sc1cccc(S[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 370.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	7.881		Crippen Method
rinpol	2273.20		NIST Webbook
rinpol	2273.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U353069&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/112-852-1/1-3-Benzenedithiol-S-S-bis-tert-butyldimethylsilyl.pdf>

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