

1,3-Benzenedimethanethiol, S,S'-bis(trimethylsilyl)-

Other names: 1,3-Benzenedimethanethiol, 2tms derivative
Inchi: InChI=1S/C14H26S2Si2/c1-17(2,3)15-11-13-8-7-9-14(10-13)12-16-18(4,5)6/h7-10H,11-13H
InchiKey: BHWMSITZTMKEAH-UHFFFAOYSA-N
Formula: C14H26S2Si2
SMILES: C[Si](C)(C)SCc1cccc(CS[Si](C)(C)C)c1
Mol. weight [g/mol]: 314.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	5.823		Crippen Method
rinsol	2050.60		NIST Webbook
rinsol	2050.60		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=U353032&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/119-877-7/1-3-Benzenedimethanethiol-S-S-bis-trimethylsilyl.pdf>

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