

1,3-Benzenedimethanethiol, S-(tert-butyldimethylsilyl)-

Other names: 1,3-Benzenedimethanethiol, tbdms derivative
Inchi: InChI=1S/C14H24S2Si/c1-14(2,3)17(4,5)16-11-13-8-6-7-12(9-13)10-15/h6-9,15H,10-11H
InchiKey: GNHQPVVVOOWVEMW-UHFFFAOYSA-N
Formula: C14H24S2Si
SMILES: CC(C)(C)[Si](C)(C)SCc1cccc(CS)c1
Mol. weight [g/mol]: 284.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	5.355		Crippen Method
rinpol	2083.90		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U353035&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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