

2,6-Dimethylbenzenethiol, S-(tert-butyldimethylsilyl)-

Other names: 2,6-Dimethylbenzenethiol, tbdms derivative
Inchi: InChI=1S/C14H24SSi/c1-11-9-8-10-12(2)13(11)15-16(6,7)14(3,4)5/h8-10H,1-7H3
InchiKey: IXQUBWAWDIZMTB-UHFFFAOYSA-N
Formula: C14H24SSi
SMILES: Cc1cccc(C)c1S[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 252.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	5.401		Crippen Method
rinpol	1678.50		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U353024&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/68-623-5/2-6-Dimethylbenzenethiol-S-tert-butyldimethylsilyl.pdf>

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