3-Methylbenzenethiol, S-(tert-butyldimethylsilyl)-

Other names: 3-Methylbenzenethiol, tbdms derivative

Inchi: InChI=1S/C13H22SSi/c1-11-8-7-9-12(10-11)14-15(5,6)13(2,3)4/h7-10H,1-6H3

InchiKey: BYPIKEILDWPHQH-UHFFFAOYSA-N

Formula: C13H22SSi

SMILES: Cc1cccc(S[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 238.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	5.092		Crippen Method
rinpol	1575.40		NIST Webbook
rinpol	1575.40		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=U353005&Units=SI

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/93-177-3/3-Methylbenzenethiol-S-tert-butyldimethylsilyl.pdf

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