

3-(Methylthio)benzoic acid, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C14H22O2SSi/c1-14(2,3)18(5,6)16-13(15)11-8-7-9-12(10-11)17-4/h7-10H,1-6H
InchiKey: XMFPVBVKORTSOZ-UHFFFAOYSA-N
Formula: C14H22O2SSi
SMILES: CSc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 282.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	4.571		Crippen Method
rinpol	1905.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374604&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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