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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices