

# 4-(Methylthio)benzoic acid, tert.-butyldimethylsilyl ester

**Inchi:** InChI=1S/C14H22O2SSi/c1-14(2,3)18(5,6)16-13(15)11-7-9-12(17-4)10-8-11/h7-10H,1-6H  
**InchiKey:** TXRZHXSDOTZOGY-UHFFFAOYSA-N  
**Formula:** C14H22O2SSi  
**SMILES:** CSc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1  
**Mol. weight [g/mol]:** 282.47

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	4.571		Crippen Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374606&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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