2-(Methylthio)benzoic acid, trimethylsilyl ester

Inchi: InChI=1S/C11H16O2SSi/c1-14-10-8-6-5-7-9(10)11(12)13-15(2,3)4/h5-8H,1-4H3
InchiKey: VKUGICGAHXDAAO-UHFFFAOYSA-N
Formula: C11H16O2SSi
SMILES: CSc1ccccc1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 240.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	3.400		Crippen Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		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=U374603&Units=SI

Legend

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