Thiosalicylic acid, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C13H20O2SSi/c1-13(2,3)17(4,5)15-12(14)10-8-6-7-9-11(10)16/h6-9,16H,1-5H
InchiKey: KEEAXGFXJXIFEX-UHFFFAOYSA-N
Formula: C13H20O2SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1S
Mol. weight [g/mol]: 268.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	4.137		Crippen Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374598&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