4-Mercaptobenzoic acid, S-trimethylsilyl-, trimethylsilyl ester

Other names: 4-Mercaptobenzoic acid, 2tms derivative
Inchi: InChI=1S/C13H22O2SSi2/c1-17(2,3)15-13(14)11-7-9-12(10-8-11)16-18(4,5)6/h7-10H,1-6
InchiKey: PLEILNHUYGIMSA-UHFFFAOYSA-N
Formula: C13H22O2SSi2
SMILES: C[Si](C)(C)OC(=O)c1ccc(S[Si](C)(C)C)cc1
Mol. weight [g/mol]: 298.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	4.605		Crippen Method
rinpol	1795.00		NIST Webbook
rinpol	1801.80		NIST Webbook
rinpol	1801.80		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=U352983&Units=SI

Legend

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