3-Mercaptobenzoic acid, S-trimethylsilyl-, trimethylsilyl ester

Other names: 3-Mercaptobenzoic acid, 2tms derivative

Inchi: InChI=1S/C13H22O2SSi2/c1-17(2,3)15-13(14)11-8-7-9-12(10-11)16-18(4,5)6/h7-10H,1-6

InchiKey: BWXOAADEYNKOEC-UHFFFAOYSA-N

Formula: C13H22O2SSi2

SMILES: C[Si](C)(C)OC(=O)c1cccc(S[Si](C)(C)C)c1

Mol. weight [g/mol]: 298.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	4.605		Crippen Method
rinpol	1738.00		NIST Webbook
rinpol	1743.70		NIST Webbook
rinpol	1743.70		NIST Webbook
rinpol	1738.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352987&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

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