

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:	BWXOAADEYNKOEK-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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352987&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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