

Thiosalicylic acid, S-trimethylsilyl-, trimethylsilyl ester

Other names: Thiosalicylic acid, 2tms derivative
Inchi: InChI=1S/C13H22O2SSi2/c1-17(2,3)15-13(14)11-9-7-8-10-12(11)16-18(4,5)6/h7-10H,1-6
InchiKey: BYCZOPBRJLQLGV-UHFFFAOYSA-N
Formula: C13H22O2SSi2
SMILES: C[Si](C)(C)OC(=O)c1ccccc1S[Si](C)(C)C
Mol. weight [g/mol]: 298.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.23		Crippen Method
logp	4.605		Crippen Method
rinpol	1678.00		NIST Webbook
rinpol	1683.40		NIST Webbook
rinpol	1683.40		NIST Webbook
rinpol	1678.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352979&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/114-262-4/Thiosalicylic-acid-S-trimethylsilyl-trimethylsilyl-ester.pdf>

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