

5-(Methylthio)salicylic acid, trimethylsilyl ester

Inchi: InChI=1S/C11H16O3SSi/c1-15-8-5-6-10(12)9(7-8)11(13)14-16(2,3)4/h5-7,12H,1-4H3
InchiKey: MTHWODCTOZKQKB-UHFFFAOYSA-N
Formula: C11H16O3SSi
SMILES: CSc1ccc(O)c(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]: 256.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.89		Crippen Method
logp	3.106		Crippen Method
rinsol	1730.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374254&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/62-569-2/5-Methylthio-salicylic-acid-trimethylsilyl-ester.pdf>

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