Benzoic acid, 3-acetylthio-, trimethylsilyl ester

Inchi: InChI=1S/C12H16O3SSi/c1-9(13)16-11-7-5-6-10(8-11)12(14)15-17(2,3)4/h5-8H,1-4H3
InchiKey: NJLWCBFCICHNCF-UHFFFAOYSA-N
Formula: C12H16O3SSi
SMILES: CC(=O)Sc1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]: 268.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	3.317		Crippen Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		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=U375177&Units=SI

Legend

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