Benzoic acid, 4-acetylthio-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C15H22O3SSi/c1-11(16)19-13-9-7-12(8-10-13)14(17)18-20(5,6)15(2,3)4/h7-10

InchiKey: SIBUMQXHAYPRAQ-UHFFFAOYSA-N

Formula: C15H22O3SSi

SMILES: CC(=O)Sc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 310.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	4.487		Crippen Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375184&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices