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

Inchi: InChI=1S/C15H19F3O3SSi/c1-14(2,3)23(4,5)21-12(19)10-6-8-11(9-7-10)22-13(20)15(16
InchiKey: QCPFBHPSCWKMLZ-UHFFFAOYSA-N
Formula: C15H19F3O3SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 364.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	5.030		Crippen Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		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=U375183&Units=SI

Legend

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