Benzoic acid, 2-pentafluoropropionylthio-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C16H19F5O3SSi/c1-14(2,3)26(4,5)24-12(22)10-8-6-7-9-11(10)25-13(23)15(17

InchiKey: RDUIIDQTASIGGK-UHFFFAOYSA-N

Formula: C16H19F5O3SSi

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 414.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	5.665		Crippen Method
rinpol	1720.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375197&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