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

Inchi: InChI=1S/C17H19F7O3SSi/c1-14(2,3)29(4,5)27-12(25)10-6-8-11(9-7-10)28-13(26)15(18

InchiKey: IJFWVOTYOSSYGA-UHFFFAOYSA-N

Formula: C17H19F7O3SSi

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 464.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	6.300		Crippen Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		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=U375181&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices