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

Inchi: InChI=1S/C16H19F5O4Si/c1-14(2,3)26(4,5)25-12(22)10-6-8-11(9-7-10)24-13(23)15(17,1

InchiKey: SMAUJVYWNYJJCY-UHFFFAOYSA-N

Formula: C16H19F5O4Si

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

Mol. weight [g/mol]: 398.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	4.952		Crippen Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375042&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices