4-Aminobenzoic acid, N,N-bis(pentafluoropropionyl)-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C19H19F10NO4Si/c1-15(2,3)35(4,5)34-12(31)10-6-8-11(9-7-10)30(13(32)16(2

InchiKey: JXSNMOWCOBVCLX-UHFFFAOYSA-N

Formula: C19H19F10NO4Si

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

Mol. weight [g/mol]: 543.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	6.103		Crippen Method
rinpol	1642.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375092&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