4-Aminobenzoic acid, N-pentafluoropropionyl-, trimethylsilyl ester

Inchi: InChI=1S/C13H14F5NO3Si/c1-23(2,3)22-10(20)8-4-6-9(7-5-8)19-11(21)12(14,15)13(16,1

InchiKey: ZRKGFXPLGMPQDP-UHFFFAOYSA-N

Formula: C13H14F5NO3Si

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

Mol. weight [g/mol]: 355.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	3.814		Crippen Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375126&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