4-Aminobenzoic acid, N,N-bis(-trifluoroacetyl)-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F6NO4Si/c1-26(2,3)25-10(22)8-4-6-9(7-5-8)21(11(23)13(15,16)17)12(

InchiKey: BYBDEQLGVDSXML-UHFFFAOYSA-N

Formula: C14H13F6NO4Si

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

Mol. weight [g/mol]: 401.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	3.662		Crippen Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375129&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