2-Aminobenzoic acid, N- trifluoroacetyl -, N,O-bis(tert.-butyldimethylsilyl)-

Inchi: InChI=1S/C21H34F3NO3Si2/c1-19(2,3)29(7,8)25(18(27)21(22,23)24)16-14-12-11-13-15

InchiKey: FXYNVAHELHQAAO-UHFFFAOYSA-N

Formula: C21H34F3NO3Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1N(C(=O)C(F)(F)F)[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 461.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	6.749		Crippen Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375104&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