3-Aminobenzoic acid, N,N-bis(acetyl)-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C17H25NO4Si/c1-12(19)18(13(2)20)15-10-8-9-14(11-15)16(21)22-23(6,7)17(3

InchiKey: HBQSJFUKHFQKJX-UHFFFAOYSA-N

Formula: C17H25NO4Si

SMILES: CC(=O)N(C(C)=O)c1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 335.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	3.748		Crippen Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375087&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