N-Acetyl-L-phenylalanine, tert-butyldimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl N-acetylphenylalaninate
N-acetyl-l-phenylalanine, tbdms derivative

Inchi: InChI=1S/C17H27NO3Si/c1-13(19)18-15(12-14-10-8-7-9-11-14)16(20)21-22(5,6)17(2,3)4

InchiKey: VINKUEAJNUHJPG-UHFFFAOYSA-N

Formula: C17H27NO3Si

SMILES: CC(=O)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	3.282		Crippen Method
rinpol	2052.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332877&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices