tert-Butyldimethylsilyl N-(4-aminobenzoyl)glycinate

Other names: 2.4-Aminohippuric acid, tert-butyldimethylsilyl ester
Hippuric acid, p-amino-, tert-butyldimethylsilyl ester
para-Aminohippuric acid, tert-butyldimethylsilyl ester
tert-Butyldimethylsilyl 2-[(4-aminobenzoyl)amino]acetate

Inchi: InChI=1S/C15H24N2O3Si/c1-15(2,3)21(4,5)20-13(18)10-17-14(19)11-6-8-12(16)9-7-11/h

InchiKey: SADNVUGOUAJKDM-UHFFFAOYSA-N

Formula: C15H24N2O3Si

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

Mol. weight [g/mol]: 308.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	2.547		Crippen Method
rinpol	2646.00		NIST Webbook
rinpol	2646.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373406&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