3-Phenylpropionyl glycine, TBDMS

Inchi: InChI=1S/C17H27NO3Si/c1-17(2,3)22(4,5)21-16(20)13-18-15(19)12-11-14-9-7-6-8-10-14
InchiKey: AXDCGVNEJFEIDY-UHFFFAOYSA-N
Formula: C17H27NO3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CNC(=O)CCc1ccccc1
Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	3.284		Crippen Method
rinpol	2263.00		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=R563636&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices