Phenylpropionylglycine, TMS # 2

Inchi: InChI=1S/C17H29NO3Si2/c1-8-16(20-22(2,3)4)18(15-12-10-9-11-13-15)14-17(19)21-23(
InchiKey: FKCWHNSWJVLCIA-PXNMLYILSA-N
Formula: C17H29NO3Si2
SMILES: CC=C(O[Si](C)(C)C)N(CC(=O)O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]: 351.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.04		Crippen Method
logp	4.584		Crippen Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401395&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