Phenylpropionylglycine, TMS # 1

Inchi: InChI=1S/C14H21NO3Si/c1-5-13(16)15(12-9-7-6-8-10-12)11-14(17)18-19(2,3)4/h6-10H,
InchiKey: ZAGVQHZEJKLQHM-UHFFFAOYSA-N
Formula: C14H21NO3Si
SMILES: CCC(=O)N(CC(=O)O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]: 279.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.58		Crippen Method
logp	2.808		Crippen Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401380&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