Valeryl acetyl glycine, TMS # 3

Inchi: InChI=1S/C15H31NO4Si2/c1-9-10-11-14(17)16(13(2)19-21(3,4)5)12-15(18)20-22(6,7)8/h
InchiKey: RRTIEYHFAREHMF-UHFFFAOYSA-N
Formula: C15H31NO4Si2
SMILES: C=C(O[Si](C)(C)C)N(CC(=O)O[Si](C)(C)C)C(=O)CCCC
Mol. weight [g/mol]: 345.58

Physical Properties

Property code	Value	Unit	Source
log10ws	0.66		Crippen Method
logp	3.706		Crippen Method
rinpol	1515.00		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=R401706&Units=SI

Legend

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