Octanoylglycine TBDMS

Inchi: InChI=1S/C22H47NO3Si2/c1-12-13-14-15-16-17-19(25-27(8,9)21(2,3)4)23-18-20(24)26-
InchiKey: IAAADWMWODDUTJ-NMWGTECJSA-N
Formula: C22H47NO3Si2
SMILES: CCCCCCCC(=NCC(=O)O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 429.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	7.316		Crippen Method
rinpol	2076.00		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=R277122&Units=SI

Legend

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