Biotin, TMS

Inchi: InChI=1S/C15H30N2O3SSi2/c1-22(2,3)19-13(18)9-7-8-12-14-11(10-21-12)16-15(17-14)2
InchiKey: VRTYBBSNSFHHIZ-YRGRVCCFSA-N
Formula: C15H30N2O3SSi2
SMILES: C[Si](C)(C)OC(=O)CCCC1SCC2N=C(O[Si](C)(C)C)NC21
Mol. weight [g/mol]: 374.65

Physical Properties

Property code	Value	Unit	Source
log10ws	0.49		Crippen Method
logp	3.198		Crippen Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R400743&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