

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)
InchiKey: VRTYBBSNSFHIZ-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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/17-617-8/Biotin-TMS.pdf>

Generated by Cheméo on 2024-04-30 03:22:17.255194356 +0000 UTC m=+16736586.175771720.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.