Pentanoic acid, 3-hydroxy-2-propyl, bis-TMS

Other names: 2-Propyl-3-hydroxypentanoic acid, diTMS
2-propyl-3-hydroxy-pentanoic acid, TMS
Inchi: InChI=1S/C14H32O3Si2/c1-9-11-12(14(15)17-19(6,7)8)13(10-2)16-18(3,4)5/h12-13H,9-1
InchiKey: ZQFAKXFWMDHIJN-UHFFFAOYSA-N
Formula: C14H32O3Si2
SMILES: CCCC(C(=O)O[Si](C)(C)C)C(CC)O[Si](C)(C)C
Mol. weight [g/mol]: 304.57

Physical Properties

Property code	Value	Unit	Source
log10ws	0.40		Crippen Method
logp	4.411		Crippen Method
rinpol	1394.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1392.00		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=U72014&Units=SI

Legend

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