Pentanedioic acid, 2-propyl, TMS

Other names: Pentanedioic acid, 2-propyl, bis-TMS
2-Propylglutaric acid, diTMS
Inchi: InChI=1S/C14H30O4Si2/c1-8-9-12(14(16)18-20(5,6)7)10-11-13(15)17-19(2,3)4/h12H,8-1
InchiKey: MTIYPCGPTBSGLS-UHFFFAOYSA-N
Formula: C14H30O4Si2
SMILES: CCCC(CCC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 318.56

Physical Properties

Property code	Value	Unit	Source
log10ws	0.73		Crippen Method
logp	3.939		Crippen Method
rinpol	1551.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1543.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U72013&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

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