

2-n-Propyl-3-ketovalerate, bis(O-trimethylsilyl)-

Other names:

3-Oxopentanoic acid, 2-propyl, TMS

2-Propyl-3-ketopentanoic acid, diTMS

Inchi:

InChI=1S/C14H30O3Si2/c1-9-11-12(14(15)17-19(6,7)8)13(10-2)16-18(3,4)5/h9-11H2,1-8

InchiKey:

SFBVEJZEAAGDNI-SEYXRHQNSA-N

Formula:

C14H30O3Si2

SMILES:

CCCC(C(=O)O[Si](C)(C)C)=C(CC)O[Si](C)(C)C

Mol. weight [g/mol]:

302.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.08		Crippen Method
logp	4.680		Crippen Method
rinpol	1426.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1426.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U79665&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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