

Pentanoic acid, 4-oxo-2-propyl, TMS

Inchi: InChI=1S/C14H30O3Si2/c1-9-10-13(14(15)17-19(6,7)8)11-12(2)16-18(3,4)5/h11,13H,9-14H,10H,12H,14H,15H,16H,17H,18H,19H
InchiKey: GREILMJVGXHZDZ-QXMHVHEDSA-N
Formula: C14H30O3Si2
SMILES: CCCC(C=C(C)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 302.56

Physical Properties

Property code	Value	Unit	Source
log10ws	0.16		Crippen Method
logp	4.536		Crippen Method
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R168013&Units=SI>

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/23-156-3/Pentanoic-acid-4-oxo-2-propyl-TMS.pdf>

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