

4-Pentenoic acid, 2-(1-oxopropyl), enol-bis-TMS, # 2

Inchi: InChI=1S/C14H28O3Si2/c1-9-11-12(14(15)17-19(6,7)8)13(10-2)16-18(3,4)5/h9H,1,10-11H,2H
InchiKey: ANIJSCIMBKHJLX-OUKQBFOZSA-N
Formula: C14H28O3Si2
SMILES: C=CCC(C(=O)O[Si](C)(C)C)=C(CC)O[Si](C)(C)C
Mol. weight [g/mol]: 300.54

Physical Properties

Property code	Value	Unit	Source
log10ws	0.06		Crippen Method
logp	4.456		Crippen Method
rinpol	1435.00		NIST Webbook
rinpol	1435.00		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=R167887&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/121-795-5/4-Pentenoic-acid-2-1-oxopropyl-enol-bis-TMS-2.pdf>

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