Pentanoic acid, 3-oxo-2-propyl, enol-bis-TMS, # 1

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	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R167956&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