2-Pentenoic acid, 3-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Othernames: 2-Keto-3-methylvaleric acid, enol, di-TMS
2-Keto-3-methylvaleric acid, enol, (2TMS)
2-Keto-3-methylvaleric acid, enol, TMS
Inchi: InChI=1S/C12H26O3Si2/c1-9-10(2)11(14-16(3,4)5)12(13)15-17(6,7)8/h9H2,1-8H3/b11-1
InchiKey: RHJGXCQRZWTGMA-KHPPLWFESA-N
Formula: C12H26O3Si2
SMILES: CCC(C)=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 274.50
CAS: 55320-09-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpol	1325.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55320097&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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