2-Keto-3-methylvaleric acid, TMS # 2

Inchi: InChI=1S/C12H26O3Si2/c1-9-10(2)11(14-16(3,4)5)12(13)15-17(6,7)8/h9H2,1-8H3
InchiKey: RHJGXCQRZWTGMA-UHFFFAOYSA-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

Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpol	1306.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R400283&Units=SI

Legend

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