2-Keto-3-methylvaleric acid, MO TBDMS # 2

Inchi: InChI=1S/C13H27NO3Si/c1-9-10(2)11(14-16-6)12(15)17-18(7,8)13(3,4)5/h10H,9H2,1-8H
InchiKey: PDRXIEHYKBTUOD-UHFFFAOYSA-N
Formula: C13H27NO3Si
SMILES: CCC(C)C(=NOC)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 273.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.18		Crippen Method
logp	3.583		Crippen Method
rinpol	1403.00		NIST Webbook
rinpol	1403.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563116&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