2-Ketoisovaleric acid, MO TBDMS # 1

Inchi: InChI=1S/C12H25NO3Si/c1-9(2)10(13-15-6)11(14)16-17(7,8)12(3,4)5/h9H,1-8H3
InchiKey: NRDONGGIXSHQCH-UHFFFAOYSA-N
Formula: C12H25NO3Si
SMILES: CON=C(C(=O)O[Si](C)(C)C(C)(C)C)C(C)C
Mol. weight [g/mol]: 259.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	3.193		Crippen Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		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=R563210&Units=SI

Legend

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