2-Ketocaproic acid, MO TBDMS # 2

Inchi: InChI=1S/C13H27NO3Si/c1-8-9-10-11(14-16-5)12(15)17-18(6,7)13(2,3)4/h8-10H2,1-7H3
InchiKey: BTYPTKZEDRJFFP-UHFFFAOYSA-N
Formula: C13H27NO3Si
SMILES: CCCCC(=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	-1.42		Crippen Method
logp	3.727		Crippen Method
rinpol	1463.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563161&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