

2-Ketoisocaproic acid, MO TBDMS # 1

Inchi: InChI=1S/C13H27NO3Si/c1-10(2)9-11(14-16-6)12(15)17-18(7,8)13(3,4)5/h10H,9H2,1-8H
InchiKey: JTYOLYQRFAXOFR-UHFFFAOYSA-N
Formula: C13H27NO3Si
SMILES: CON=C(CC(C)C)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	1393.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R563196&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/70-889-8/2-Ketoisocaproic-acid-MO-TBDMS-1.pdf>

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