

# 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/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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