

# 2-Ketocaproic acid, TMS # 1

**Inchi:** InChI=1S/C12H26O3Si2/c1-8-9-10-11(14-16(2,3)4)12(13)15-17(5,6)7/h10H,8-9H2,1-7H3  
**InchiKey:** JZFKPTHPKLNAMQ-UHFFFAOYSA-N  
**Formula:** C12H26O3Si2  
**SMILES:** CCCC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 274.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.75		Crippen Method
logp	3.900		Crippen Method
rinpol	1308.00		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](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400312&Units=SI>

## Legend

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

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