

2-Ketovaleric acid, TMS # 2

Inchi: InChI=1S/C11H24O3Si2/c1-8-9-10(13-15(2,3)4)11(12)14-16(5,6)7/h9H,8H2,1-7H3
InchiKey: OHSILHRTQNZRQH-UHFFFAOYSA-N
Formula: C11H24O3Si2
SMILES: CCC=C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 260.48

Physical Properties

Property code	Value	Unit	Source
log10ws	1.17		Crippen Method
logp	3.510		Crippen Method
rinpol	1306.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R400416&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/118-656-3/2-Ketovaleric-acid-TMS-2.pdf>

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