

3-Ketovaleric acid, oxime, di-TMS, #1

Inchi: InChI=1S/C11H25NO3Si2/c1-8-10(12-15-17(5,6)7)9-11(13)14-16(2,3)4/h8-9H2,1-7H3/b1
InchiKey: IMFOACHXAITQFM-ZRDIBKRKSA-N
Formula: C11H25NO3Si2
SMILES: CCC(CC(=O)O[Si](C)(C)C)=NO[Si](C)(C)C
Mol. weight [g/mol]: 275.49

Physical Properties

Property code	Value	Unit	Source
log10ws	1.37		Crippen Method
logp	3.372		Crippen Method
rinsol	1306.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R51606&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/114-327-2/3-Ketovaleric-acid-oxime-di-TMS-1.pdf>

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