

Val, TMS # 2

Inchi: InChI=1S/C14H35NO2Si3/c1-12(2)13(14(16)17-20(9,10)11)15(18(3,4)5)19(6,7)8/h12-13
InchiKey: JDHOURMNSQSMHM-UHFFFAOYSA-N
Formula: C14H35NO2Si3
SMILES: CC(C)C(C(=O)O[Si](C)(C)C)N([Si](C)(C)C)[Si](C)(C)C
Mol. weight [g/mol]: 333.69

Physical Properties

Property code	Value	Unit	Source
log10ws	2.86		Crippen Method
logp	4.361		Crippen Method
rinpol	1239.00		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=R503956&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/63-999-4/Val-TMS-2.pdf>

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