

Valeryl acetyl glycine, TMS # 2

Inchi: InChI=1S/C15H31NO4Si2/c1-9-10-11-14(19-21(3,4)5)16(13(2)17)12-15(18)20-22(6,7)8/H
InchiKey: BGACNZHYXXCLRL-KAMYIIQDSA-N
Formula: C15H31NO4Si2
SMILES: CCCC=C(O[Si](C)(C)C)N(CC(=O)O[Si](C)(C)C)C(C)=O
Mol. weight [g/mol]: 345.58

Physical Properties

Property code	Value	Unit	Source
log10ws	0.66		Crippen Method
logp	3.706		Crippen Method
rinpol	1494.00		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=R401697&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/124-706-0/Valeryl-acetyl-glycine-TMS-2.pdf>

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