

Valeryl acetyl glycine, TMS # 1

Inchi: InChI=1S/C12H23NO4Si/c1-6-7-8-11(15)13(10(2)14)9-12(16)17-18(3,4)5/h6-9H2,1-5H3
InchiKey: JPZJRDYTKUARDX-UHFFFAOYSA-N
Formula: C12H23NO4Si
SMILES: CCCCC(=O)N(CC(=O)O[Si](C)(C)C)C(C)=O
Mol. weight [g/mol]: 273.40

Physical Properties

Property code	Value	Unit	Source
log10ws	0.12		Crippen Method
logp	1.930		Crippen Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook

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=R401682&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/93-771-3/Valeryl-acetyl-glycine-TMS-1.pdf>

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