L-Proline, N-pivaloyl-, isohexyl ester

Inchi: InChI=1S/C16H29NO3/c1-12(2)8-7-11-20-14(18)13-9-6-10-17(13)15(19)16(3,4)5/h12-13
InchiKey: KZQVBYIOOGOOQR-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: CC(C)CCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	3.003		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346358&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.