

L-Proline, N-pivaloyl-, pentyl ester

Inchi: InChI=1S/C15H27NO3/c1-5-6-7-11-19-13(17)12-9-8-10-16(12)14(18)15(2,3)4/h12H,5-11H
InchiKey: JEBNKZRPYVOMRV-UHFFFAOYSA-N
Formula: C15H27NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	2.757		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346357&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

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<https://www.chemeo.com/cid/91-232-3/L-Proline-N-pivaloyl-pentyl-ester.pdf>

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