L-Proline, N-pivaloyl-, ethyl ester

Inchi: InChI=1S/C12H21NO3/c1-5-16-10(14)9-7-6-8-13(9)11(15)12(2,3)4/h9H,5-8H2,1-4H3
InchiKey: CPXLUDFDHAUOKT-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: CCOC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	1.587		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook

Sources

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=U346355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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