

L-Phe-L-Pro lactam

Inchi: InChI=1S/C14H16N2O2/c17-13-12-7-4-8-16(12)14(18)11(15-13)9-10-5-2-1-3-6-10/h1-3,5-8,11-13,16-18/t17-18/m1
InchiKey: QZBUWPVZSXDWSB-NWDGAFQWSA-N
Formula: C14H16N2O2
SMILES: O=C1NC(Cc2ccccc2)C(=O)N2CCCC12
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.718		Crippen Method
mcvol	185.740	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R14505&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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