

L-Proline, N-(p-anisoyl)-, methyl ester

Inchi: InChI=1S/C14H17NO4/c1-18-11-7-5-10(6-8-11)13(16)15-9-3-4-12(15)14(17)19-2/h5-8,12
InchiKey: OCNAZFCOCMJDDJO-UHFFFAOYSA-N
Formula: C14H17NO4
SMILES: COC(=O)C1CCCN1C(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 263.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	1.473		Crippen Method
mcvol	198.360	ml/mol	McGowan Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U299671&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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