

I-Proline, N-(m-toluoyl)-, methyl ester

Inchi:	InChI=1S/C14H17NO3/c1-10-5-3-6-11(9-10)13(16)15-8-4-7-12(15)14(17)18-2/h3,5-6,9,1
InchiKey:	QZCQSCWQKLPTLU-UHFFFAOYSA-N
Formula:	C14H17NO3
SMILES:	<chem>COC(=O)C1CCCN1C(=O)c1cccc(C)c1</chem>
Mol. weight [g/mol]:	247.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.773		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	1992.00		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=U299640&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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