l-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: COC(=O)C1CCCN1C(=O)c1cccc(C)c1
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/ci990307l
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