l-Proline, N-(p-toluoyl)-, methyl ester

Inchi: InChI=1S/C14H17NO3/c1-10-5-7-11(8-6-10)13(16)15-9-3-4-12(15)14(17)18-2/h5-8,12H,
InchiKey: NVQUYGQMRCNVOJ-UHFFFAOYSA-N
Formula: C14H17NO3
SMILES: COC(=O)C1CCCN1C(=O)c1ccc(C)cc1
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	2018.00		NIST Webbook
rinpol	2018.00		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=U299650&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.