l-Proline, N-(O-anisoyl)-, methyl ester

Inchi: InChI=1S/C14H17NO4/c1-18-12-8-4-3-6-10(12)13(16)15-9-5-7-11(15)14(17)19-2/h3-4,6,
InchiKey: RWDILUJUMDRMPX-UHFFFAOYSA-N
Formula: C14H17NO4
SMILES: COC(=O)C1CCCN1C(=O)c1ccccc1OC
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	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299754&Units=SI
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

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.