5-Oxo-1-phenylacetyl-pyrrolidine-2-carboxylic acid methyl ester

Other names: 5-Oxoproline, N-(phenylacetyl), methyl ester
Inchi: InChI=1S/C14H15NO4/c1-19-14(18)11-7-8-12(16)15(11)13(17)9-10-5-3-2-4-6-10/h2-6,1
InchiKey: ODDCKAZQWSFWLA-UHFFFAOYSA-N
Formula: C14H15NO4
SMILES: COC(=O)C1CCC(=O)N1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 261.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	0.920		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook

Sources

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=R106411&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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