L-Proline, N-(phenylacetyl)-, ethyl ester

Inchi: InChI=1S/C15H19NO3/c1-2-19-15(18)13-9-6-10-16(13)14(17)11-12-7-4-3-5-8-12/h3-5,7-
InchiKey: WQCLPYDTKCAQPT-UHFFFAOYSA-N
Formula: C15H19NO3
SMILES: CCOC(=O)C1CCCN1C(=O)Cc1ccccc1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.783		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346189&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

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