L-Proline, N-(3-methoxybenzoyl)-, ethyl ester

Inchi: InChI=1S/C15H19NO4/c1-3-20-15(18)13-8-5-9-16(13)14(17)11-6-4-7-12(10-11)19-2/h4,6
InchiKey: ZBEVKWZYKDMAIC-UHFFFAOYSA-N
Formula: C15H19NO4
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 277.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.863		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346166&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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