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

Inchi: InChI=1S/C15H19NO3/c1-3-19-15(18)13-8-5-9-16(13)14(17)12-7-4-6-11(2)10-12/h4,6-7,
InchiKey: XKAKRDMVBGASPC-UHFFFAOYSA-N
Formula: C15H19NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.163		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		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=U346251&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.