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

Inchi: InChI=1S/C16H21NO3/c1-3-10-20-16(19)14-8-5-9-17(14)15(18)13-7-4-6-12(2)11-13/h4,6
InchiKey: PBPOHMHICPJDES-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	2.553		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		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=U346252&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.