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

Inchi: InChI=1S/C17H23NO3/c1-3-4-11-21-17(20)15-9-6-10-18(15)16(19)14-8-5-7-13(2)12-14/l
InchiKey: WEHNQKOYSYMKOH-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)c1cccc(C)c1
Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	2.943		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346253&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.