l-Proline, N-(4-butylbenzoyl)-, methyl ester

Inchi: InChI=1S/C17H23NO3/c1-3-4-6-13-8-10-14(11-9-13)16(19)18-12-5-7-15(18)17(20)21-2/l
InchiKey: WXUPAZIYYXZGDA-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: CCCCc1ccc(C(=O)N2CCCC2C(=O)OC)cc1
Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	2.807		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		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=U299695&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.