L-Proline, N-(4-butylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C18H25NO3/c1-3-5-7-14-9-11-15(12-10-14)17(20)19-13-6-8-16(19)18(21)22-4
InchiKey: PADJIZAEYUVZHX-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: CCCCc1ccc(C(=O)N2CCCC2C(=O)OCC)cc1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	3.197		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		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=U346271&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.