

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

Inchi: InChI=1S/C19H27NO3/c1-3-5-7-15-9-11-16(12-10-15)18(21)20-13-6-8-17(20)19(22)23-1
InchiKey: VRMPKLJINLXJNN-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CCCCc1ccc(C(=O)N2CCCC2C(=O)OCCC)cc1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.587		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346272&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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