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

Inchi: InChI=1S/C21H31NO3/c1-3-5-7-16-25-21(24)19-10-8-15-22(19)20(23)18-13-11-17(12-14
InchiKey: FUVVLENERDXFRW-UHFFFAOYSA-N
Formula: C21H31NO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	4.367		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346273&Units=SI
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

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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