L-Proline, N-(4-ethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C26H41NO3/c1-3-5-6-7-8-9-10-11-12-13-21-30-26(29)24-15-14-20-27(24)25(2
InchiKey: GQVAVFIPUGFLRK-UHFFFAOYSA-N
Formula: C26H41NO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 415.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	6.318		Crippen Method
mcvol	361.570	ml/mol	McGowan Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook

Sources

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=U346270&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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