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

Inchi: InChI=1S/C20H29NO3/c1-4-16-9-11-17(12-10-16)19(22)21-13-5-8-18(21)20(23)24-14-6-

InchiKey: WRZFRLFMJLVBLP-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: CCc1ccc(C(=O)N2CCCC2C(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	3.833		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346268&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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