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

Inchi: InChI=1S/C16H21NO3/c1-3-12-7-9-13(10-8-12)15(18)17-11-5-6-14(17)16(19)20-4-2/h7-1
InchiKey: WUUUKVSONRYEQL-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	2.417		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346267&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.