L-Proline, N-(4-fluorobenzoyl)-, heptyl ester

Inchi: InChI=1S/C19H26FNO3/c1-2-3-4-5-6-14-24-19(23)17-8-7-13-21(17)18(22)15-9-11-16(20
InchiKey: JUQUIYDQAULLTF-UHFFFAOYSA-N
Formula: C19H26FNO3
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 335.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.944		Crippen Method
mcvol	264.710	ml/mol	McGowan Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346127&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.