L-Proline, N-(2-fluorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C24H36FNO3/c1-2-3-4-5-6-7-8-9-10-13-19-29-24(28)22-17-14-18-26(22)23(27
InchiKey: HKMQSOKUPGVZHS-UHFFFAOYSA-N
Formula: C24H36FNO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1F
Mol. weight [g/mol]: 405.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.894		Crippen Method
mcvol	335.160	ml/mol	McGowan Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		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=U346102&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

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