

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

Inchi:	InChI=1S/C27H42FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-32-27(31)25-20-17-21-29
InchiKey:	DHXUXUOUDPSMAN-UHFFFAOYSA-N
Formula:	C27H42FNO3
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1F
Mol. weight [g/mol]:	447.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	7.065		Crippen Method
mcvol	377.430	ml/mol	McGowan Method
rinpol	3359.00		NIST Webbook
rinpol	3359.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U346104&Units=SI

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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