

L-Proline, N-(2,4-difluorobenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C24H35F2NO3/c1-2-3-4-5-6-7-8-9-10-11-17-30-24(29)22-13-12-16-27(22)23(2)
InchiKey:	LCROFVYAFQSCCR-UHFFFAOYSA-N
Formula:	C24H35F2NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)cc1F
Mol. weight [g/mol]:	423.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	6.034		Crippen Method
mcvol	336.930	ml/mol	McGowan Method
rinsol	2948.00		NIST Webbook
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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=U346043&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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