

L-Proline, N-(3,4-difluorobenzoyl)-, hexadecyl ester

Inchi:	InChI=1S/C28H43F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-34-28(33)26-17-16-2
InchiKey:	ATAVCKHDSCERIR-UHFFFAOYSA-N
Formula:	C28H43F2NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	479.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.10		Crippen Method
logp	7.594		Crippen Method
mcvol	393.290	ml/mol	McGowan Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		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=U345915&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

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<https://www.chemeo.com/cid/123-047-3/L-Proline-N-3-4-difluorobenzoyl-hexadecyl-ester.pdf>

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