

L-Proline, N-(2,6-difluorobenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C28H43F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-34-28(33)25-20-17-21
InchiKey: OIABTQPWMXIFNM-UHFFFAOYSA-N
Formula: C28H43F2NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1F
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	3446.00		NIST Webbook
rinpol	3446.00		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=U346404&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/115-282-1/L-Proline-N-2-6-difluorobenzoyl-hexadecyl-ester.pdf>

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