

Isonipecotic acid, N-(3,4-difluorobenzoyl)-, undecyl ester

Inchi:	InChI=1S/C24H35F2NO3/c1-2-3-4-5-6-7-8-9-10-17-30-24(29)19-13-15-27(16-14-19)23(2
InchiKey:	RKZKPZLZXRKZTR-UHFFFAOYSA-N
Formula:	C24H35F2NO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
Mol. weight [g/mol]:	423.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.07		Crippen Method
logp	5.891		Crippen Method
mcvol	336.930	ml/mol	McGowan Method
rinpola	3140.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361273&Units=SI

Legend

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

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