

Isonipecotic acid, N-(2,4-difluorobenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C25H37F2NO3/c1-2-3-4-5-6-7-8-9-10-11-18-31-25(30)20-14-16-28(17-15-20)2
InchiKey:	ISFFYLUHALMLKJ-UHFFFAOYSA-N
Formula:	C25H37F2NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1
Mol. weight [g/mol]:	437.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.49		Crippen Method
logp	6.281		Crippen Method
mcvol	351.020	ml/mol	McGowan Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361375&Units=SI
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

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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