Isonipecotic acid, N-(2,6-difluoro-3-methylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C25H37F2NO3/c1-3-4-5-6-7-8-9-10-11-18-31-25(30)20-14-16-28(17-15-20)24(

InchiKey: QDAVBCMMOWIPJV-UHFFFAOYSA-N

Formula: C25H37F2NO3

SMILES: CCCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1

Mol. weight [g/mol]: 437.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.55		Crippen Method
logp	6.199		Crippen Method
mcvol	351.020	ml/mol	McGowan Method
rinpol	3245.00		NIST Webbook
rinpol	3245.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361304&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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