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

Inchi: InChI=1S/C19H25F2NO3/c1-3-4-5-12-25-19(24)14-8-10-22(11-9-14)18(23)16-15(20)7-6-

InchiKey: JFQJEBQSCGJWAX-UHFFFAOYSA-N

Formula: C19H25F2NO3

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

Mol. weight [g/mol]: 353.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	3.859		Crippen Method
mcvol	266.480	ml/mol	McGowan Method
rinpol	2608.00		NIST Webbook

Sources

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

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=U361301&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices