

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

Inchi:	InChI=1S/C19H25F2NO3/c1-13(2)4-3-11-25-19(24)14-7-9-22(10-8-14)18(23)15-5-6-16(2
InchiKey:	BIENEWFVGKKEGU-UHFFFAOYSA-N
Formula:	C19H25F2NO3
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
Mol. weight [g/mol]:	353.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.796		Crippen Method
mcvol	266.480	ml/mol	McGowan Method
rinpol	2566.00		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=U361267&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

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