

Isonipecotic acid, N-(2,5-difluorobenzoyl)-, ethyl ester

Inchi:	InChI=1S/C15H17F2NO3/c1-2-21-15(20)10-5-7-18(8-6-10)14(19)12-9-11(16)3-4-13(12)1
InchiKey:	HTQJHASWBIVCMU-UHFFFAOYSA-N
Formula:	C15H17F2NO3
SMILES:	CCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]:	297.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	2.380		Crippen Method
mcvol	210.120	ml/mol	McGowan Method
rinpola	2152.00		NIST Webbook

Sources

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=U361408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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