

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

Inchi:	InChI=1S/C18H23F2NO3/c1-2-3-4-11-24-18(23)13-7-9-21(10-8-13)17(22)15-12-14(19)5
InchiKey:	XYAOKKIXQJYPPR-UHFFFAOYSA-N
Formula:	C18H23F2NO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]:	339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	3.550		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpole	2472.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361412&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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