

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

Inchi:	InChI=1S/C16H19F2NO3/c1-2-9-22-16(21)11-5-7-19(8-6-11)15(20)13-10-12(17)3-4-14(1)
InchiKey:	LTXZCFLVNZBCEC-UHFFFAOYSA-N
Formula:	C16H19F2NO3
SMILES:	CCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]:	311.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.770		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
rinpola	2261.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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