

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

Inchi:	InChI=1S/C21H29F2NO3/c1-2-3-4-5-6-7-14-27-21(26)16-10-12-24(13-11-16)20(25)17-8
InchiKey:	NBNYYHWMGGLQGZ-UHFFFAOYSA-N
Formula:	C21H29F2NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
Mol. weight [g/mol]:	381.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.82		Crippen Method
logp	4.721		Crippen Method
mcvol	294.660	ml/mol	McGowan Method
rinpola	2807.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices

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