

Isonipecotinoylisonipecotic acid, N'-(2,5-difluorobenzoyl)-, isobutyl ester

Inchi: InChI=1S/C23H30F2N2O4/c1-15(2)14-31-23(30)17-7-11-26(12-8-17)21(28)16-5-9-27(10)
InchiKey: NELJVXUQUTZKPA-UHFFFAOYSA-N
Formula: C23H30F2N2O4
SMILES: CC(C)COC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(F)ccc3F)CC2)CC1
Mol. weight [g/mol]: 436.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.255		Crippen Method
mcvol	323.530	ml/mol	McGowan Method
rmpol	3525.00		NIST Webbook
rmpol	3525.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361428&Units=SI>

Legend

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

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