

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

Inchi: InChI=1S/C21H26F2N2O4/c1-2-29-21(28)15-7-11-24(12-8-15)19(26)14-5-9-25(10-6-14)
InchiKey: ZERUEWCIMQNHPPZ-UHFFFAOYSA-N
Formula: C21H26F2N2O4
SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(F)ccc3F)CC2)CC1
Mol. weight [g/mol]: 408.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	2.619		Crippen Method
mcvol	295.350	ml/mol	McGowan Method
rinsol	3337.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361426&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinsol: Non-polar retention indices

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