Isonipecotinoylisonipecotic acid, N'-(3,4-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: WBKCNUKHXRKCBH-UHFFFAOYSA-N

Formula: C21H26F2N2O4

SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)c(F)c3)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
rinpol	3361.00		NIST Webbook
rinpol	3361.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361280&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.