Isonipecotic acid, N-(3-fluorobenzoyl)-, ethyl ester

Inchi: InChI=1S/C15H18FNO3/c1-2-20-15(19)11-6-8-17(9-7-11)14(18)12-4-3-5-13(16)10-12/h3

InchiKey: NNBJXMMSNYUVRG-UHFFFAOYSA-N

Formula: C15H18FNO3

SMILES: CCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1

Mol. weight [g/mol]: 279.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	2.241		Crippen Method
mcvol	208.350	ml/mol	McGowan Method
rinpol	2196.00		NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.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=U361521&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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