

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/40-664-0/Isonipecotic-acid-N-3-fluorobenzoyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-24 04:28:37.183639288 +0000 UTC m=+16222166.104216612.

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