

Isonipecotic acid, N-(4-fluorobenzoyl)-, pentyl ester

Inchi:	InChI=1S/C18H24FNO3/c1-2-3-4-13-23-18(22)15-9-11-20(12-10-15)17(21)14-5-7-16(19)
InchiKey:	MHCAYCOBXZPVBR-UHFFFAOYSA-N
Formula:	C18H24FNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	321.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.411		Crippen Method
mcvol	250.620	ml/mol	McGowan Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361071&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
rinpol:	Non-polar retention indices

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