

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

Inchi:	InChI=1S/C19H26FNO3/c1-14(2)4-3-13-24-19(23)16-9-11-21(12-10-16)18(22)15-5-7-17
InchiKey:	QEGVJHJDWCPLQV-UHFFFAOYSA-N
Formula:	C19H26FNO3
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	335.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.657		Crippen Method
mcvol	264.710	ml/mol	McGowan Method
rinpola	2588.00		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=U361072&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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