

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

Inchi:	InChI=1S/C25H38FNO3/c1-2-3-4-5-6-7-8-9-10-11-20-30-25(29)22-16-18-27(19-17-22)24
InchiKey:	ABVHZDAZKUJIAZ-UHFFFAOYSA-N
Formula:	C25H38FNO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	419.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	6.142		Crippen Method
mcvol	349.250	ml/mol	McGowan Method
rinsol	3269.00		NIST Webbook
rinsol	3269.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361079&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
rinsol:	Non-polar retention indices

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