

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

Inchi:	InChI=1S/C23H34FNO3/c1-2-3-4-5-6-7-8-9-17-28-23(27)19-13-15-25(16-14-19)22(26)20
InchiKey:	SULVIZQDLDRWBK-UHFFFAOYSA-N
Formula:	C23H34FNO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]:	391.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.362		Crippen Method
mcvol	321.070	ml/mol	McGowan Method
rinpol	3056.00		NIST Webbook

Sources

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=U361526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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