

# Isonipectic acid, N-(3-fluorobenzoyl)-, nonyl ester

Inchi:	InChI=1S/C22H32FNO3/c1-2-3-4-5-6-7-8-16-27-22(26)18-12-14-24(15-13-18)21(25)19-1
InchiKey:	GCMGEDOURWXFGW-UHFFFAOYSA-N
Formula:	C22H32FNO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]:	377.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	4.972		Crippen Method
mcvol	306.980	ml/mol	McGowan Method
rmpol	2947.00		NIST Webbook
rmpol	2947.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361525&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361525&amp;Units=SI</a>

## Legend

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

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