

Isonipectic acid, N-(3-fluorobenzoyl)-, octyl ester

Inchi:	InChI=1S/C21H30FNO3/c1-2-3-4-5-6-7-15-26-21(25)17-11-13-23(14-12-17)20(24)18-9-8
InchiKey:	QUBSLEGITFWMEI-UHFFFAOYSA-N
Formula:	C21H30FNO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]:	363.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	4.582		Crippen Method
mcvol	292.890	ml/mol	McGowan Method
rinsol	2829.00		NIST Webbook
rinsol	2829.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361524&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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