

Isonipecotic acid, N-(2-chlorobenzoyl)-, nonyl ester

Inchi:	InChI=1S/C22H32ClNO3/c1-2-3-4-5-6-7-10-17-27-22(26)18-13-15-24(16-14-18)21(25)19
InchiKey:	DSIOWQNMOSTISL-UHFFFAOYSA-N
Formula:	C22H32ClNO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]:	393.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	5.486		Crippen Method
mcvol	317.450	ml/mol	McGowan Method
rmpol	3148.00		NIST Webbook
rmpol	3148.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361164&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
rmpol:	Non-polar retention indices

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