

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

Inchi:	InChI=1S/C18H24ClNO3/c1-2-3-6-13-23-18(22)14-9-11-20(12-10-14)17(21)15-7-4-5-8-1
InchiKey:	DGBXATPAETYCJT-UHFFFAOYSA-N
Formula:	C18H24ClNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]:	337.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	3.926		Crippen Method
mcvol	261.090	ml/mol	McGowan Method
rinsol	2703.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361159&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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