

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

Inchi:	InChI=1S/C19H26ClNO3/c1-2-3-4-7-14-24-19(23)15-10-12-21(13-11-15)18(22)16-8-5-6-
InchiKey:	MLLWMKNCLAFBEY-UHFFFAOYSA-N
Formula:	C19H26ClNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]:	351.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	4.316		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
rmpol	2809.00		NIST Webbook
rmpol	2809.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361161&Units=SI

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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