

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

Inchi:	InChI=1S/C16H20ClNO3/c1-2-11-21-16(20)12-7-9-18(10-8-12)15(19)13-5-3-4-6-14(13)1
InchiKey:	RNIZPTOOPLECFU-UHFFFAOYSA-N
Formula:	C16H20ClNO3
SMILES:	CCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]:	309.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	3.145		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
rinpol	2495.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=U361156&Units=SI

Legend

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

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