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: RNIZPTOOPLECFL-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/ci990307l

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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