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

Inchi: InChI=1S/C17H22ClNO3/c1-2-3-12-22-17(21)13-8-10-19(11-9-13)16(20)14-6-4-5-7-15(1

InchiKey: ZBRGBDOMGDZPOG-UHFFFAOYSA-N

Formula: C17H22ClNO3

SMILES: CCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1

Mol. weight [g/mol]: 323.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.536		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
rinpol	2601.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361158&Units=SI

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

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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