

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

Inchi: InChI=1S/C15H18ClNO3/c1-2-20-15(19)11-7-9-17(10-8-11)14(18)12-5-3-4-6-13(12)16/h
InchiKey: UQMRCDVKEQKZDB-UHFFFAOYSA-N
Formula: C15H18ClNO3
SMILES: CCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 295.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.755		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
rinpol	2383.00		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=U361155&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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