

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

Inchi: InChI=1S/C17H22ClNO3/c1-12(2)11-22-17(21)13-7-9-19(10-8-13)16(20)14-5-3-4-6-15(1)
InchiKey: FGTLJFLPYZJMHR-UHFFFAOYSA-N
Formula: C17H22ClNO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 323.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	3.391		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361157&Units=SI>
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>

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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