

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
rinpola	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/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
rinpola:	Non-polar retention indices

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