Isonipecotic acid, N-(3-chloropropionyl)-, ethyl ester

Inchi: InChI=1S/C11H18ClNO3/c1-2-16-11(15)9-4-7-13(8-5-9)10(14)3-6-12/h9H,2-8H2,1H3

InchiKey: RQAVOJRSNJZSIB-UHFFFAOYSA-N

Formula: C11H18ClNO3

SMILES: CCOC(=O)C1CCN(C(=O)CCCl)CC1

Mol. weight [g/mol]: 247.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	1.417		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
rinpol	1876.00		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=U360941&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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