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

Inchi: InChI=1S/C14H24ClNO3/c1-2-3-4-11-19-14(18)12-6-9-16(10-7-12)13(17)5-8-15/h12H,2-

InchiKey: CFSLYBBHKRZHEU-UHFFFAOYSA-N

Formula: C14H24ClNO3

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

Mol. weight [g/mol]: 289.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.587		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		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=U360944&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.