Isonipecotic acid, N-(5-chlorovaleryl)-, isohexyl ester

Inchi: InChI=1S/C17H30ClNO3/c1-14(2)6-5-13-22-17(21)15-8-11-19(12-9-15)16(20)7-3-4-10-1

InchiKey: OTQJYMXMTBSYQF-UHFFFAOYSA-N

Formula: C17H30ClNO3

SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)CCCCCl)CC1

Mol. weight [g/mol]: 331.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.613		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2617.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361007&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices