

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

Inchi:	InChI=1S/C13H22ClNO3/c1-2-18-13(17)11-6-9-15(10-7-11)12(16)5-3-4-8-14/h11H,2-10H
InchiKey:	KQCDBWOUOZINJO-UHFFFAOYSA-N
Formula:	C13H22ClNO3
SMILES:	CCOC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]:	275.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	2.197		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
rinpola	2233.00		NIST Webbook

Sources

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=U361002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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