

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

Inchi:	InChI=1S/C17H30ClNO3/c1-2-3-4-7-14-22-17(21)15-9-12-19(13-10-15)16(20)8-5-6-11-1
InchiKey:	MDCBAFWRNURPEY-UHFFFAOYSA-N
Formula:	C17H30ClNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]:	331.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	3.758		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2654.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361008&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

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