

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

Inchi:	InChI=1S/C16H28ClNO3/c1-2-3-6-13-21-16(20)14-8-11-18(12-9-14)15(19)7-4-5-10-17/h
InchiKey:	XDXBSDOHKODNZ-UHFFFAOYSA-N
Formula:	C16H28ClNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]:	317.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.367		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
rinpola	2553.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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