

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

Inchi:	InChI=1S/C18H32ClNO3/c1-2-3-4-5-8-15-23-18(22)16-10-13-20(14-11-16)17(21)9-6-7-1
InchiKey:	UWROHKPUEGWUHP-UHFFFAOYSA-N
Formula:	C18H32ClNO3
SMILES:	CCCCCCCOC(=O)C1CCN(C(=O)CCCCCl)CC1
Mol. weight [g/mol]:	345.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	4.148		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
rinpola	2753.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361009&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvola:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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