Isonipecotic acid, N-(3-chloropropionyl)-, nonyl ester

Inchi: InChI=1S/C18H32ClNO3/c1-2-3-4-5-6-7-8-15-23-18(22)16-10-13-20(14-11-16)17(21)9-12-19/h16H,2-15H2,1H3

InchiKey: MXMOBAZWHYULPG-UHFFFAOYSA-N

Formula: C18H32ClNO3

SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)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
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360948&Units=SI

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

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.