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

Inchi: InChI=1S/C22H40ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-27-22(26)20-14-17-24(18-15-2

InchiKey: JUGKDPCQHIHHCP-UHFFFAOYSA-N

Formula: C22H40ClNO3

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1

Mol. weight [g/mol]: 402.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.05		Crippen Method
logp	5.708		Crippen Method
mcvol	341.210	ml/mol	McGowan Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360952&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

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