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

Inchi: InChI=1S/C23H42ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-28-23(27)21-15-18-25(19-1

InchiKey: TVMTXMCISXDFTF-UHFFFAOYSA-N

Formula: C23H42ClNO3

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

Mol. weight [g/mol]: 416.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	6.098		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360953&Units=SI

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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