

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

Inchi: InChI=1S/C20H36ClNO3/c1-2-3-4-5-6-7-8-9-10-17-25-20(24)18-12-15-22(16-13-18)19(2)
InchiKey: TZESQTHBSMGXRE-UHFFFAOYSA-N
Formula: C20H36ClNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]: 373.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.928		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		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=U360950&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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