

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

Inchi:	InChI=1S/C21H38ClNO3/c1-2-3-4-5-6-7-8-9-10-11-18-26-21(25)19-13-16-23(17-14-19)2
InchiKey:	SFBKBAVJTGDZPM-UHFFFAOYSA-N
Formula:	C21H38ClNO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]:	387.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	5.318		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
rinpol	2936.00		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=U360951&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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