

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

Inchi:	InChI=1S/C24H44ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-29-24(28)22-16-19-26(2
InchiKey:	GJOQTAUMPRJABY-UHFFFAOYSA-N
Formula:	C24H44ClNO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]:	430.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	6.488		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
rinpola	3255.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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