

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:	CCCCCCCCCCCCCOC(=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
rinsol	3152.00		NIST Webbook
rinsol	3152.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/60-565-8/Isonipecotic-acid-N-3-chloropropionyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-20 06:16:20.272898925 +0000 UTC m=+15883029.193476240.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.