

Isonipectic acid, N-(3-chloropropionyl)-, decyl ester

Inchi: InChI=1S/C19H34ClNO3/c1-2-3-4-5-6-7-8-9-16-24-19(23)17-11-14-21(15-12-17)18(22)1
InchiKey: GTFRIZHRPVYTCX-UHFFFAOYSA-N
Formula: C19H34ClNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1
Mol. weight [g/mol]: 359.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	4.538		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
rinpol	2717.00		NIST Webbook
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Sources

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=U360949&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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