

Isonipectic acid, N-(2-chlorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H36ClNO3/c1-2-3-4-5-6-7-8-9-12-19-29-24(28)20-15-17-26(18-16-20)23(2)
InchiKey: PPLVDXHWLNHAFP-UHFFFAOYSA-N
Formula: C24H36ClNO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2Cl)CC1
Mol. weight [g/mol]: 422.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	6.266		Crippen Method
mcvol	345.630	ml/mol	McGowan Method
rinsol	3358.00		NIST Webbook
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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=U361166&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

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