

# Isonipectic acid, N-(3-chloropropionyl)-, tridecyl ester

**Inchi:** InChI=1S/C22H40ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-27-22(26)20-14-17-24(18-15-2  
**InchiKey:** JUGKDPCQHIIHCP-UHFFFAOYSA-N  
**Formula:** C22H40ClNO3  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CCCl)CC1  
**Mol. weight [g/mol]:** 402.01

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.05   |        | Crippen Method |
| logp          | 5.708   |        | Crippen Method |
| mcvol         | 341.210 | ml/mol | McGowan Method |
| rinsol        | 3046.00 |        | NIST Webbook   |
| rinsol        | 3046.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](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=U360952&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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