# Isonipecotic acid, N-(5-chlorovaleryl)-, heptyl ester

**Inchi:** InChI=1S/C18H32ClNO3/c1-2-3-4-5-8-15-23-18(22)16-10-13-20(14-11-16)17(21)9-6-7-1

**InchiKey:** UWROHKPUEGWUHP-UHFFFAOYSA-N

**Formula:** C18H32ClNO3

**SMILES:** CCCCCCCOC(=O)C1CCN(C(=O)CCCCCl)CC1

**Mol. weight [g/mol]:** 345.90

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.37 | | Crippen Method |
| logp | 4.148 | | Crippen Method |
| mcvol | 284.850 | ml/mol | McGowan Method |
| rinpol | 2753.00 | | NIST Webbook |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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=U361009&Units=SI

## 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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