

# Isonipecotic acid, N-ethoxycarbonyl-, isoheptyl ester

**Inchi:** InChI=1S/C15H27NO4/c1-4-19-15(18)16-9-7-13(8-10-16)14(17)20-11-5-6-12(2)3/h12-13  
**InchiKey:** KZWDHPVWMDROBU-UHFFFAOYSA-N  
**Formula:** C15H27NO4  
**SMILES:** CCOC(=O)N1CCC(C(=O)OCCCC(C)C)CC1  
**Mol. weight [g/mol]:** 285.38

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.79   |        | Crippen Method |
| logp          | 2.834   |        | Crippen Method |
| mcvol         | 236.210 | ml/mol | McGowan Method |
| rinpol        | 2032.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U322005&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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