

# Isonipecotic acid, N-propoxycarbonyl-, isobutyl ester

**Inchi:** InChI=1S/C14H25NO4/c1-4-9-18-14(17)15-7-5-12(6-8-15)13(16)19-10-11(2)3/h11-12H,4  
**InchiKey:** KXTCEVIFVKMRPQ-UHFFFAOYSA-N  
**Formula:** C14H25NO4  
**SMILES:** CCCOC(=O)N1CCC(C(=O)OCC(C)C)CC1  
**Mol. weight [g/mol]:** 271.36

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 2.444   |        | Crippen Method |
| mcvol         | 222.120 | ml/mol | McGowan Method |
| rinpol        | 1939.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Cheméo Relay (1.0):**  
**Cheméo Relay (1.0, beta):**  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322076&Units=SI>  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## Legend

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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