

# d-Proline, N-isobutoxycarbonyl-, hexadecyl ester

**Inchi:** InChI=1S/C26H49NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-30-25(28)24-19-18-2  
**InchiKey:** FZFWYLRVYUKYGQ-UHFFFAOYSA-N  
**Formula:** C26H49NO4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C  
**Mol. weight [g/mol]:** 439.67

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.74   |        | Crippen Method |
| logp          | 7.268   |        | Crippen Method |
| mcvol         | 391.200 | ml/mol | McGowan Method |
| rinpol        | 2836.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320815&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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