

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

**Inchi:** InChI=1S/C27H51NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-31-26(29)25-20-1  
**InchiKey:** UZYQJWIBERCEDT-UHFFFAOYSA-N  
**Formula:** C27H51NO4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C  
**Mol. weight [g/mol]:** 453.70

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.16		Crippen Method
logp	7.658		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
rinpol	2970.00		NIST Webbook

## Sources

**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=U320816&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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