

# d-Proline, n-butoxycarbonyl-, heptyl ester

**Inchi:** InChI=1S/C17H31NO4/c1-3-5-7-8-9-14-21-16(19)15-11-10-12-18(15)17(20)22-13-6-4-2/  
**InchiKey:** APETUAKJTJTKOY-UHFFFAOYSA-N  
**Formula:** C17H31NO4  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)OCCCC  
**Mol. weight [g/mol]:** 313.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	3.901		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321085&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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