

# L-Proline, N-(5-bromovaleryl)-, hexyl ester

**Inchi:** InChI=1S/C16H28BrNO3/c1-2-3-4-7-13-21-16(20)14-9-8-12-18(14)15(19)10-5-6-11-17/h  
**InchiKey:** KMXUKZISXJWKNW-UHFFFAOYSA-N  
**Formula:** C16H28BrNO3  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)CCCCBr  
**Mol. weight [g/mol]:** 362.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	3.666		Crippen Method
mcvol	261.930	ml/mol	McGowan Method
rinpol	2522.00		NIST Webbook
rinpol	2522.00		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=U346050&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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