

# Pipecolylpipecolic acid, N-butoxycarbonyl-, hexyl ester

**Inchi:** InChI=1S/C23H40N2O5/c1-3-5-7-12-18-29-22(27)20-14-9-10-15-24(20)21(26)19-13-8-1  
**InchiKey:** QHPQMPDBKAYRBD-UHFFFAOYSA-N  
**Formula:** C23H40N2O5  
**SMILES:** CCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCCCC  
**Mol. weight [g/mol]:** 424.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	4.282		Crippen Method
mcvol	349.620	ml/mol	McGowan Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393067&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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