

# Pipecolylpipecolic acid, N-butoxycarbonyl-, octyl ester

**Inchi:** InChI=1S/C25H44N2O5/c1-3-5-7-8-9-14-20-31-24(29)22-16-11-12-17-26(22)23(28)21-15  
**InchiKey:** GKYGEGYTYPFXIU-UHFFFAOYSA-N  
**Formula:** C25H44N2O5  
**SMILES:** CCCCCCOC(=O)C1CCCN1C(=O)C1CCCN1C(=O)OCCCC  
**Mol. weight [g/mol]:** 452.63

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.92   |        | Crippen Method |
| logp          | 5.062   |        | Crippen Method |
| mcvol         | 377.800 | ml/mol | McGowan Method |
| rinpole       | 3108.00 |        | NIST Webbook   |
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## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393069&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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