

# Pipecolylpipecolic acid, N-butoxycarbonyl-, butyl ester

<b>Inchi:</b>	InChI=1S/C21H36N2O5/c1-3-5-15-27-20(25)18-12-8-9-13-22(18)19(24)17-11-7-10-14-23
<b>InchiKey:</b>	WFYHJQUXZLBDSL-UHFFFAOYSA-N
<b>Formula:</b>	C21H36N2O5
<b>SMILES:</b>	CCCCOC(=O)C1CCCCN1C(=O)C1CCCCN1C(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	396.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.502		Crippen Method
mcvol	321.440	ml/mol	McGowan Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393065&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393065&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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