

# Benzethidine

<b>Other names:</b>	4-Piperidinecarboxylic acid, 4-phenyl-1-[2-(phenylmethoxy)ethyl]-, ethyl ester Isonipécotic acid, 1-[2-(benzyloxy)ethyl]-4-phenyl-, ethyl ester Benzethidin NIH 7574 Ethyl 1-(2-benzyloxyethyl)-4-phenylpiperidine-4-carboxylate 1-(2-Benzyloxyethyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester
<b>Inchi:</b>	InChI=1S/C23H29NO3/c1-2-27-22(25)23(21-11-7-4-8-12-21)13-15-24(16-14-23)17-18-20
<b>InchiKey:</b>	UVTBZAWTRVBTMK-UHFFFAOYSA-N
<b>Formula:</b>	C23H29NO3
<b>SMILES:</b>	CCOC(=O)C1(c2ccccc2)CCN(CCOCc2ccccc2)CC1
<b>Mol. weight [g/mol]:</b>	367.48
<b>CAS:</b>	3691-78-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.800		Crippen Method
mcvol	299.840	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3691789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3691789&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>
<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>

## 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

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