

# «beta»-Alanine, N-(2-furoyl)-, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C22H37NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-27-21(24)16-17-23-22(25)20-
<b>InchiKey:</b>	DGRQNCHAZMSADD-UHFFFAOYSA-N
<b>Formula:</b>	C22H37NO4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1cccc1
<b>Mol. weight [g/mol]:</b>	379.53

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.11		Crippen Method
logp	5.644		Crippen Method
mcvol	326.240	ml/mol	McGowan Method
rinpola	3004.00		NIST Webbook
rinpola	3004.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321983&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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
<b>rinpola:</b>	Non-polar retention indices

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