

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

**Inchi:** InChI=1S/C24H41NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-29-23(26)18-19-25-24(27)17  
**InchiKey:** IIHOTSMHQPEAHK-UHFFFAOYSA-N  
**Formula:** C<sub>24</sub>H<sub>41</sub>NO<sub>4</sub>  
**SMILES:** CCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccco1  
**Mol. weight [g/mol]:** 407.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.95		Crippen Method
logp	6.424		Crippen Method
mcvol	354.420	ml/mol	McGowan Method
rinpol	3415.00		NIST Webbook
rinpol	3415.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.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=U321985&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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