

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

**Inchi:** InChI=1S/C15H23NO4/c1-2-3-4-5-6-11-20-14(17)9-10-16-15(18)13-8-7-12-19-13/h7-8,12-14,17-18,20  
**InchiKey:** LJSKWCDSWXAVRG-UHFFFAOYSA-N  
**Formula:** C15H23NO4  
**SMILES:** CCCCCCOC(=O)CCNC(=O)c1ccco1  
**Mol. weight [g/mol]:** 281.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.18		Crippen Method
logp	2.913		Crippen Method
mcvol	227.610	ml/mol	McGowan Method
rinpole	2195.00		NIST Webbook
rinpole	2195.00		NIST Webbook

## 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=U321977&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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