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

Inchi: InChI=1S/C13H19NO4/c1-2-3-4-9-18-12(15)7-8-14-13(16)11-6-5-10-17-11/h5-6,10H,2-4
InchiKey: ADSIWGUADDAHGY-UHFFFAOYSA-N
Formula: C13H19NO4
SMILES: CCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 253.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	2.133		Crippen Method
mcvol	199.430	ml/mol	McGowan Method
rinpol	1999.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321975&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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