

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

Inchi:	InChI=1S/C23H39NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-28-22(25)17-18-24-23(26)
InchiKey:	GBLBRRRRZYIBF-UHFFFAOYSA-N
Formula:	C23H39NO4
SMILES:	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]:	393.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.53		Crippen Method
logp	6.034		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
rinpola	3156.00		NIST Webbook
rinpola	3156.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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