

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

Inchi: InChI=1S/C14H21NO4/c1-11(2)5-3-10-19-13(16)7-8-15-14(17)12-6-4-9-18-12/h4,6,9,11H
InchiKey: XOJCTWFEQUCDMO-UHFFFAOYSA-N
Formula: C14H21NO4
SMILES: CC(C)CCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.52		Crippen Method
logp	2.379		Crippen Method
mcvol	213.520	ml/mol	McGowan Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321976&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

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