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

Inchi: InChI=1S/C12H17NO4/c1-9(2)8-17-11(14)5-6-13-12(15)10-4-3-7-16-10/h3-4,7,9H,5-6,8H
InchiKey: DUJXKNDAYXOJQV-UHFFFAOYSA-N
Formula: C12H17NO4
SMILES: CC(C)COC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 239.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	1.599		Crippen Method
mcvol	185.340	ml/mol	McGowan Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook

Sources

Crippen Method: 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=U321973&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.