

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

Inchi: InChI=1S/C10H13NO4/c1-2-14-9(12)5-6-11-10(13)8-4-3-7-15-8/h3-4,7H,2,5-6H2,1H3,(H
InchiKey: AXHJMKIGTFSKMC-UHFFFAOYSA-N
Formula: C10H13NO4
SMILES: CCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 211.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	0.963		Crippen Method
mcvol	157.160	ml/mol	McGowan Method
rinpol	1693.00		NIST Webbook
rinpol	1693.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321971&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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