

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

Inchi: InChI=1S/C11H15NO4/c1-2-7-16-10(13)5-6-12-11(14)9-4-3-8-15-9/h3-4,8H,2,5-7H2,1H3
InchiKey: SKWYUEGZBIRNNI-UHFFFAOYSA-N
Formula: C11H15NO4
SMILES: CCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 225.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.51		Crippen Method
logp	1.353		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321972&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

Latest version available from:

<https://www.cheméo.com/cid/30-566-0/beta-Alanine-N-2-furoyl-propyl-ester.pdf>

Generated by Cheméo on 2025-12-05 15:55:46.285030027 +0000 UTC m=+4698343.815070682.

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