

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

Inchi: InChI=1S/C18H29NO4/c1-2-3-4-5-6-7-8-9-14-23-17(20)12-13-19-18(21)16-11-10-15-22-
InchiKey: HESZVMGDTAYKIM-UHFFFAOYSA-N
Formula: C18H29NO4
SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 323.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.44		Crippen Method
logp	4.083		Crippen Method
mcvol	269.880	ml/mol	McGowan Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		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=U321980&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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<https://www.chemeo.com/cid/97-626-0/beta-Alanine-N-2-furoyl-decyl-ester.pdf>

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