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

Inchi: InChI=1S/C16H25NO4/c1-2-3-4-5-6-7-12-21-15(18)10-11-17-16(19)14-9-8-13-20-14/h8-9
InchiKey: QYQOFSCZYCYYCH-UHFFFAOYSA-N
Formula: C16H25NO4
SMILES: CCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 295.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	3.303		Crippen Method
mcvol	241.700	ml/mol	McGowan Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		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=U321978&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

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