

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

Inchi: InChI=1S/C17H27NO4/c1-2-3-4-5-6-7-8-13-22-16(19)11-12-18-17(20)15-10-9-14-21-15/
InchiKey: RMVYTNXUEKCFNU-UHFFFAOYSA-N
Formula: C17H27NO4
SMILES: CCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.02		Crippen Method
logp	3.693		Crippen Method
mcvol	255.790	ml/mol	McGowan Method
rinpol	2410.00		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=U321979&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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