

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

Inchi: InChI=1S/C19H31NO4/c1-2-3-4-5-6-7-8-9-10-15-24-18(21)13-14-20-19(22)17-12-11-16-
InchiKey: AWBKNSXKIJPGIF-UHFFFAOYSA-N
Formula: C19H31NO4
SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.85		Crippen Method
logp	4.474		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
rinpola	2613.00		NIST Webbook
rinpola	2613.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U321981&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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