

L-Valine, N-(2-furoyl)-, undecyl ester

Inchi: InChI=1S/C21H35NO4/c1-4-5-6-7-8-9-10-11-12-15-26-21(24)19(17(2)3)22-20(23)18-14-
InchiKey: WWZLCYXTNJSOPU-UHFFFAOYSA-N
Formula: C21H35NO4
SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1ccco1)C(C)C
Mol. weight [g/mol]: 365.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.56		Crippen Method
logp	5.108		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
rinsol	2602.00		NIST Webbook
rinsol	2602.00		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=U346697&Units=SI>

Legend

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

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