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

Inchi: InChI=1S/C24H41NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-29-24(27)22(20(2)3)25-23(
InchiKey: UVOAVKKLEJFZHC-UHFFFAOYSA-N
Formula: C24H41NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccco1)C(C)C
Mol. weight [g/mol]: 407.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.82		Crippen Method
logp	6.278		Crippen Method
mcvol	354.420	ml/mol	McGowan Method
rinpol	2898.00		NIST Webbook
rinpol	2898.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U346698&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.