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

Inchi: InChI=1S/C25H43NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-30-25(28)23(21(2)3)26-
InchiKey: JUTXAXZQNOWNLP-UHFFFAOYSA-N
Formula: C25H43NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccco1)C(C)C
Mol. weight [g/mol]: 421.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.668		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
rinpol	3012.00		NIST Webbook
rinpol	3012.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346699&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.