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

Inchi: InChI=1S/C27H47NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-32-27(30)25(23(2
InchiKey: POBCWABEYHYDDY-UHFFFAOYSA-N
Formula: C27H47NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccco1)C(C)C
Mol. weight [g/mol]: 449.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.07		Crippen Method
logp	7.449		Crippen Method
mcvol	396.690	ml/mol	McGowan Method
rinpol	3219.00		NIST Webbook
rinpol	3219.00		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=U346701&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.