

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

Inchi:	InChI=1S/C28H49NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-33-28(31)26(2
InchiKey:	WYWZXFVLZIEWHS-UHFFFAOYSA-N
Formula:	C28H49NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccco1)C(C)C
Mol. weight [g/mol]:	463.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.49		Crippen Method
logp	7.839		Crippen Method
mcvol	410.780	ml/mol	McGowan Method
rinpol	3325.00		NIST Webbook
rinpol	3325.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U346702&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

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