L-Valine, N-(3-cyclopentylpropionyl)-, undecyl ester

Inchi: InChI=1S/C24H45NO3/c1-4-5-6-7-8-9-10-11-14-19-28-24(27)23(20(2)3)25-22(26)18-17-
InchiKey: UIKTYHKYFFSJKS-UHFFFAOYSA-N
Formula: C24H45NO3
SMILES: CCCCCCCCCCCOC(=O)C(N=C(O)CCC1CCCC1)C(C)C
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
hf	-813.37	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	7.012		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	1007.95	K	Joback Method
tc	1236.16	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346659&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature