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

Inchi: InChI=1S/C25H47NO3/c1-4-5-6-7-8-9-10-11-12-15-20-29-25(28)24(21(2)3)26-23(27)19-
InchiKey: KTNZZZXSKLSMAV-UHFFFAOYSA-N
Formula: C25H47NO3
SMILES: CCCCCCCCCCCCOC(=O)C(N=C(O)CCC1CCCC1)C(C)C
Mol. weight [g/mol]: 409.65

Physical Properties

Property code	Value	Unit	Source
hf	-834.01	kJ/mol	Joback Method
hvap	99.95	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.402		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook
tb	1030.83	K	Joback Method
tc	1266.99	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346660&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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