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

Inchi: InChI=1S/C18H33NO3/c1-4-5-8-13-22-18(21)17(14(2)3)19-16(20)12-11-15-9-6-7-10-15/h14-15,17H,4-13H2,1-3H3,(H,19,20)/t17-/m0/s1

InchiKey: PQNAJFIGWOKABP-UHFFFAOYSA-N

Formula: C18H33NO3

SMILES: CCCCCOC(=O)C(N=C(O)CCC1CCCC1)C(C)C

Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
hf	-689.53	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.671		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	870.67	K	Joback Method
tc	1073.48	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346656&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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