l-Valine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C14H25NO3/c1-10(2)13(14(17)18-3)15-12(16)9-8-11-6-4-5-7-11/h10-11,13H,4

InchiKey: GWMQERYZEILNGH-UHFFFAOYSA-N

Formula: C14H25NO3

SMILES: COC(=O)C(NC(=O)CCC1CCCC1)C(C)C

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-174.78	kJ/mol	Joback Method
hf	-586.28	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.271		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1836.00		NIST Webbook
tb	714.45	K	Joback Method
tc	917.44	K	Joback Method
tf	403.19	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.11	J/mol×K	714.45	Joback Method
cpg	661.58	J/mol×K	748.28	Joback Method
cpg	677.96	J/mol×K	782.11	Joback Method
cpg	693.29	J/mol×K	815.95	Joback Method
cpg	707.58	J/mol×K	849.78	Joback Method
cpg	720.88	J/mol×K	883.61	Joback Method
cpg	733.20	J/mol×K	917.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299652&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume