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

Inchi: InChI=1S/C17H31NO3/c1-12(2)11-21-17(20)16(13(3)4)18-15(19)10-9-14-7-5-6-8-14/h12
InchiKey: VXMFHAIWAMMATP-UHFFFAOYSA-N
Formula: C17H31NO3
SMILES: CC(C)COC(=O)C(NC(=O)CCC1CCCC1)C(C)C
Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-151.96	kJ/mol	Joback Method
hf	-653.48	kJ/mol	Joback Method
hfus	32.64	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.297		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
pc	1569.72	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	782.65	K	Joback Method
tc	983.75	K	Joback Method
tf	422.00	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.44	J/mol×K	782.65	Joback Method
cpg	834.71	J/mol×K	816.17	Joback Method
cpg	851.78	J/mol×K	849.68	Joback Method
cpg	867.70	J/mol×K	883.20	Joback Method
cpg	882.51	J/mol×K	916.72	Joback Method
cpg	896.24	J/mol×K	950.23	Joback Method
cpg	908.92	J/mol×K	983.75	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=U346654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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