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

Inchi: InChI=1S/C17H31NO3/c1-4-5-12-21-17(20)16(13(2)3)18-15(19)11-10-14-8-6-7-9-14/h13

InchiKey: JLGZFRVLJPBFFM-UHFFFAOYSA-N

Formula: C17H31NO3

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

Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
gf	-149.52	kJ/mol	Joback Method
hf	-648.20	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.441		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	783.09	K	Joback Method
tc	981.74	K	Joback Method
tf	437.00	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.94	J/mol×K	783.09	Joback Method
cpg	833.98	J/mol×K	816.20	Joback Method
cpg	850.87	J/mol×K	849.31	Joback Method
cpg	866.64	J/mol×K	882.42	Joback Method
cpg	881.33	J/mol×K	915.53	Joback Method
cpg	894.98	J/mol×K	948.64	Joback Method
cpg	907.62	J/mol×K	981.74	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=U346655&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