L-Valine, N-(4-methylbenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H25NO3/c1-11(2)10-21-17(20)15(12(3)4)18-16(19)14-8-6-13(5)7-9-14/h6-9
InchiKey: IYFWXGBAESKOBP-UHFFFAOYSA-N
Formula: C17H25NO3
SMILES: Cc1ccc(C(=O)NC(C(=O)OCC(C)C)C(C)C)cc1
Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-85.73	kJ/mol	Joback Method
hf	-488.90	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	77.55	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.949		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	799.03	K	Joback Method
tc	1009.97	K	Joback Method
tf	450.04	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.97	J/mol×K	799.03	Joback Method
cpg	750.63	J/mol×K	834.19	Joback Method
cpg	765.16	J/mol×K	869.34	Joback Method
cpg	778.59	J/mol×K	904.50	Joback Method
cpg	790.97	J/mol×K	939.66	Joback Method
cpg	802.33	J/mol×K	974.81	Joback Method
cpg	812.69	J/mol×K	1009.97	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=U346639&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