l-Valine, N-(p-toluoyl)-, methyl ester

Inchi: InChI=1S/C14H19NO3/c1-9(2)12(14(17)18-4)15-13(16)11-7-5-10(3)6-8-11/h5-9,12H,1-4
InchiKey: ZNSMVFOPAMKWML-UHFFFAOYSA-N
Formula: C14H19NO3
SMILES: COC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-108.55	kJ/mol	Joback Method
hf	-421.70	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.922		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1894.00		NIST Webbook
tb	730.83	K	Joback Method
tc	945.60	K	Joback Method
tf	431.23	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.21	J/mol×K	730.83	Joback Method
cpg	582.84	J/mol×K	766.63	Joback Method
cpg	596.46	J/mol×K	802.42	Joback Method
cpg	609.09	J/mol×K	838.22	Joback Method
cpg	620.76	J/mol×K	874.01	Joback Method
cpg	631.49	J/mol×K	909.81	Joback Method
cpg	641.31	J/mol×K	945.60	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=U299647&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