l-Valine, N-(4-fluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H16FNO3/c1-8(2)11(13(17)18-3)15-12(16)9-4-6-10(14)7-5-9/h4-8,11H,1-3
InchiKey: JGANSNPTJWFOGK-UHFFFAOYSA-N
Formula: C13H16FNO3
SMILES: COC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 253.27

Physical Properties

Property code	Value	Unit	Source
gf	-311.78	kJ/mol	Joback Method
hf	-597.17	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	1.753		Crippen Method
mcvol	191.030	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	707.22	K	Joback Method
tc	916.55	K	Joback Method
tf	420.55	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.91	J/mol×K	707.22	Joback Method
cpg	536.52	J/mol×K	742.11	Joback Method
cpg	549.21	J/mol×K	777.00	Joback Method
cpg	561.00	J/mol×K	811.89	Joback Method
cpg	571.92	J/mol×K	846.78	Joback Method
cpg	581.98	J/mol×K	881.67	Joback Method
cpg	591.20	J/mol×K	916.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299605&Units=SI
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

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