L-Valine, N-(4-fluorobenzoyl)-, ethyl ester

Inchi: InChI=1S/C14H18FNO3/c1-4-19-14(18)12(9(2)3)16-13(17)10-5-7-11(15)8-6-10/h5-9,12H
InchiKey: FQAVWOBLTQWDDZ-UHFFFAOYSA-N
Formula: C14H18FNO3
SMILES: CCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 267.30

Physical Properties

Property code	Value	Unit	Source
gf	-303.36	kJ/mol	Joback Method
hf	-617.81	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	70.44	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.143		Crippen Method
mcvol	205.120	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	730.10	K	Joback Method
tc	936.88	K	Joback Method
tf	431.82	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.02	J/mol×K	730.10	Joback Method
cpg	590.04	J/mol×K	764.56	Joback Method
cpg	603.10	J/mol×K	799.03	Joback Method
cpg	615.23	J/mol×K	833.49	Joback Method
cpg	626.47	J/mol×K	867.96	Joback Method
cpg	636.83	J/mol×K	902.42	Joback Method
cpg	646.33	J/mol×K	936.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346662&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