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

Inchi: InChI=1S/C15H20FNO3/c1-4-9-20-15(19)13(10(2)3)17-14(18)11-5-7-12(16)8-6-11/h5-8,1
InchiKey: AINAVOQEOAFYPN-UHFFFAOYSA-N
Formula: C15H20FNO3
SMILES: CCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 281.32

Physical Properties

Property code	Value	Unit	Source
gf	-294.94	kJ/mol	Joback Method
hf	-638.45	kJ/mol	Joback Method
hfus	33.78	kJ/mol	Joback Method
hvap	72.67	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.533		Crippen Method
mcvol	219.210	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	752.98	K	Joback Method
tc	957.68	K	Joback Method
tf	443.09	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.29	J/mol×K	752.98	Joback Method
cpg	644.65	J/mol×K	787.10	Joback Method
cpg	658.03	J/mol×K	821.21	Joback Method
cpg	670.45	J/mol×K	855.33	Joback Method
cpg	681.96	J/mol×K	889.45	Joback Method
cpg	692.56	J/mol×K	923.57	Joback Method
cpg	702.30	J/mol×K	957.68	Joback Method

Sources

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=U346663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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