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

Inchi: InChI=1S/C16H22FNO3/c1-4-5-10-21-16(20)14(11(2)3)18-15(19)12-6-8-13(17)9-7-12/h6
InchiKey: PUYJVTRCPJHKLL-UHFFFAOYSA-N
Formula: C16H22FNO3
SMILES: CCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 295.35

Physical Properties

Property code	Value	Unit	Source
gf	-286.52	kJ/mol	Joback Method
hf	-659.09	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	74.89	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.923		Crippen Method
mcvol	233.300	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	775.86	K	Joback Method
tc	979.00	K	Joback Method
tf	454.36	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.64	J/mol×K	775.86	Joback Method
cpg	700.29	J/mol×K	809.72	Joback Method
cpg	713.94	J/mol×K	843.57	Joback Method
cpg	726.61	J/mol×K	877.43	Joback Method
cpg	738.34	J/mol×K	911.29	Joback Method
cpg	749.15	J/mol×K	945.14	Joback Method
cpg	759.07	J/mol×K	979.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346664&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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