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

Inchi: InChI=1S/C17H24FNO3/c1-4-5-6-11-22-17(21)15(12(2)3)19-16(20)13-7-9-14(18)10-8-13
InchiKey: HUFGZGSFZHYOJX-UHFFFAOYSA-N
Formula: C17H24FNO3
SMILES: CCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 309.38

Physical Properties

Property code	Value	Unit	Source
gf	-278.10	kJ/mol	Joback Method
hf	-679.73	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.313		Crippen Method
mcvol	247.390	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2142.00		NIST Webbook
rinpol	2142.00		NIST Webbook
tb	798.74	K	Joback Method
tc	1000.88	K	Joback Method
tf	465.63	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.98	J/mol×K	798.74	Joback Method
cpg	756.90	J/mol×K	832.43	Joback Method
cpg	770.78	J/mol×K	866.12	Joback Method
cpg	783.67	J/mol×K	899.81	Joback Method
cpg	795.58	J/mol×K	933.50	Joback Method
cpg	806.56	J/mol×K	967.19	Joback Method
cpg	816.64	J/mol×K	1000.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346665&Units=SI

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