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

Inchi: InChI=1S/C19H28FNO3/c1-4-5-6-7-8-13-24-19(23)17(14(2)3)21-18(22)15-9-11-16(20)12
InchiKey: PUVNOTCJDGZBKK-UHFFFAOYSA-N
Formula: C19H28FNO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 337.43

Physical Properties

Property code	Value	Unit	Source
gf	-261.26	kJ/mol	Joback Method
hf	-721.01	kJ/mol	Joback Method
hfus	44.14	kJ/mol	Joback Method
hvap	81.57	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.094		Crippen Method
mcvol	275.570	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	844.50	K	Joback Method
tc	1046.51	K	Joback Method
tf	488.17	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.36	J/mol×K	844.50	Joback Method
cpg	872.75	J/mol×K	878.17	Joback Method
cpg	887.04	J/mol×K	911.84	Joback Method
cpg	900.28	J/mol×K	945.51	Joback Method
cpg	912.50	J/mol×K	979.18	Joback Method
cpg	923.74	J/mol×K	1012.84	Joback Method
cpg	934.03	J/mol×K	1046.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346667&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