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

Inchi: InChI=1S/C21H32FNO3/c1-4-5-6-7-8-9-10-15-26-21(25)19(16(2)3)23-20(24)17-11-13-18
InchiKey: YRAPHIZKDCHGMP-UHFFFAOYSA-N
Formula: C21H32FNO3
SMILES: CCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 365.48

Physical Properties

Property code	Value	Unit	Source
gf	-244.42	kJ/mol	Joback Method
hf	-762.29	kJ/mol	Joback Method
hfus	49.32	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.874		Crippen Method
mcvol	303.750	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	890.26	K	Joback Method
tc	1094.98	K	Joback Method
tf	510.71	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.90	J/mol×K	890.26	Joback Method
cpg	991.74	J/mol×K	924.38	Joback Method
cpg	1006.42	J/mol×K	958.50	Joback Method
cpg	1019.96	J/mol×K	992.62	Joback Method
cpg	1032.43	J/mol×K	1026.74	Joback Method
cpg	1043.85	J/mol×K	1060.86	Joback Method
cpg	1054.28	J/mol×K	1094.98	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=U346669&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