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

Inchi: InChI=1S/C22H34FNO3/c1-4-5-6-7-8-9-10-11-16-27-22(26)20(17(2)3)24-21(25)18-12-14
InchiKey: JAPFVNCJEZKQKQ-UHFFFAOYSA-N
Formula: C22H34FNO3
SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1)C(C)C
Mol. weight [g/mol]: 379.51

Physical Properties

Property code	Value	Unit	Source
gf	-236.00	kJ/mol	Joback Method
hf	-782.93	kJ/mol	Joback Method
hfus	51.91	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.264		Crippen Method
mcvol	317.840	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook
tb	913.14	K	Joback Method
tc	1120.42	K	Joback Method
tf	521.98	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.20	J/mol×K	913.14	Joback Method
cpg	1052.28	J/mol×K	947.69	Joback Method
cpg	1067.15	J/mol×K	982.23	Joback Method
cpg	1080.85	J/mol×K	1016.78	Joback Method
cpg	1093.43	J/mol×K	1051.32	Joback Method
cpg	1104.93	J/mol×K	1085.87	Joback Method
cpg	1115.40	J/mol×K	1120.42	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=U346670&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