L-Valine, N-(3,4-difluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C22H33F2NO3/c1-4-5-6-7-8-9-10-11-14-28-22(27)20(16(2)3)25-21(26)17-12-1
InchiKey: NFJFIQRLAHWMGS-UHFFFAOYSA-N
Formula: C22H33F2NO3
SMILES: CCCCCCCCCCOC(=O)C(NC(=O)c1ccc(F)c(F)c1)C(C)C
Mol. weight [g/mol]: 397.50

Physical Properties

Property code	Value	Unit	Source
gf	-440.44	kJ/mol	Joback Method
hf	-990.51	kJ/mol	Joback Method
hfus	54.60	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	5.403		Crippen Method
mcvol	319.610	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	917.39	K	Joback Method
tc	1124.02	K	Joback Method
tf	535.09	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.59	J/mol×K	917.39	Joback Method
cpg	1058.35	J/mol×K	951.83	Joback Method
cpg	1072.90	J/mol×K	986.27	Joback Method
cpg	1086.27	J/mol×K	1020.71	Joback Method
cpg	1098.52	J/mol×K	1055.15	Joback Method
cpg	1109.67	J/mol×K	1089.58	Joback Method
cpg	1119.79	J/mol×K	1124.02	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=U346507&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