L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, octyl ester

Inchi: InChI=1S/C22H29F6NO3/c1-4-5-6-7-8-9-12-32-20(31)18(14(2)3)29-19(30)16-13-15(21(2
InchiKey: GUAQSMZZWDXZIZ-UHFFFAOYSA-N
Formula: C22H29F6NO3
SMILES: CCCCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C
Mol. weight [g/mol]: 469.46

Physical Properties

Property code	Value	Unit	Source
gf	-1214.00	kJ/mol	Joback Method
hf	-1792.45	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.382		Crippen Method
mcvol	326.690	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	908.01	K	Joback Method
tc	1111.70	K	Joback Method
tf	542.29	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.86	J/mol×K	908.01	Joback Method
cpg	1086.67	J/mol×K	941.96	Joback Method
cpg	1100.42	J/mol×K	975.91	Joback Method
cpg	1113.20	J/mol×K	1009.85	Joback Method
cpg	1125.09	J/mol×K	1043.80	Joback Method
cpg	1136.16	J/mol×K	1077.75	Joback Method
cpg	1146.50	J/mol×K	1111.70	Joback Method

Sources

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=U346574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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