L-Valine, N-pentafluorobenzoyl-, propyl ester

Inchi: InChI=1S/C15H16F5NO3/c1-4-5-24-15(23)13(6(2)3)21-14(22)7-8(16)10(18)12(20)11(19)
InchiKey: VPVACQKDIPIXGZ-UHFFFAOYSA-N
Formula: C15H16F5NO3
SMILES: CCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 353.28

Physical Properties

Property code	Value	Unit	Source
gf	-1112.70	kJ/mol	Joback Method
hf	-1468.77	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.090		Crippen Method
mcvol	226.290	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	769.98	K	Joback Method
tc	955.82	K	Joback Method
tf	495.53	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.07	J/mol×K	769.98	Joback Method
cpg	669.22	J/mol×K	800.95	Joback Method
cpg	680.60	J/mol×K	831.93	Joback Method
cpg	691.23	J/mol×K	862.90	Joback Method
cpg	701.10	J/mol×K	893.87	Joback Method
cpg	710.23	J/mol×K	924.85	Joback Method
cpg	718.62	J/mol×K	955.82	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=U346602&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