L-Valine, N-pentafluorobenzoyl-, isohexyl ester

Inchi: InChI=1S/C18H22F5NO3/c1-8(2)6-5-7-27-18(26)16(9(3)4)24-17(25)10-11(19)13(21)15(2

InchiKey: BTGDIXAAVJQJRD-UHFFFAOYSA-N

Formula: C18H22F5NO3

SMILES: CC(C)CCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 395.36

Physical Properties

Property code	Value	Unit	Source
gf	-1089.88	kJ/mol	Joback Method
hf	-1535.97	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	78.34	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.116		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	838.18	K	Joback Method
tc	1030.21	K	Joback Method
tf	514.34	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.06	J/mol×K	838.18	Joback Method
cpg	839.55	J/mol×K	870.18	Joback Method
cpg	852.09	J/mol×K	902.19	Joback Method
cpg	863.69	J/mol×K	934.19	Joback Method
cpg	874.36	J/mol×K	966.20	Joback Method
cpg	884.11	J/mol×K	998.20	Joback Method
cpg	892.97	J/mol×K	1030.21	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=U346606&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