L-Valine, N-pentafluorobenzoyl-, ethyl ester

Inchi: InChI=1S/C14H14F5NO3/c1-4-23-14(22)12(5(2)3)20-13(21)6-7(15)9(17)11(19)10(18)8(6
InchiKey: NNUIVGBCZUPDFL-UHFFFAOYSA-N
Formula: C14H14F5NO3
SMILES: CCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 339.26

Physical Properties

Property code	Value	Unit	Source
gf	-1121.12	kJ/mol	Joback Method
hf	-1448.13	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	2.700		Crippen Method
mcvol	212.200	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	747.10	K	Joback Method
tc	932.47	K	Joback Method
tf	484.26	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.94	J/mol×K	747.10	Joback Method
cpg	614.61	J/mol×K	777.99	Joback Method
cpg	625.57	J/mol×K	808.89	Joback Method
cpg	635.81	J/mol×K	839.78	Joback Method
cpg	645.36	J/mol×K	870.68	Joback Method
cpg	654.20	J/mol×K	901.57	Joback Method
cpg	662.34	J/mol×K	932.47	Joback Method

Sources

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=U346601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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