L-Valine, N-pentafluorobenzoyl-, butyl ester

Inchi: InChI=1S/C16H18F5NO3/c1-4-5-6-25-16(24)14(7(2)3)22-15(23)8-9(17)11(19)13(21)12(2
InchiKey: XCPRTIWVLORDNS-UHFFFAOYSA-N
Formula: C16H18F5NO3
SMILES: CCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 367.31

Physical Properties

Property code	Value	Unit	Source
gf	-1104.28	kJ/mol	Joback Method
hf	-1489.41	kJ/mol	Joback Method
hfus	47.13	kJ/mol	Joback Method
hvap	74.27	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.480		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	792.86	K	Joback Method
tc	979.78	K	Joback Method
tf	506.80	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.26	J/mol×K	792.86	Joback Method
cpg	724.86	J/mol×K	824.01	Joback Method
cpg	736.63	J/mol×K	855.17	Joback Method
cpg	747.61	J/mol×K	886.32	Joback Method
cpg	757.78	J/mol×K	917.48	Joback Method
cpg	767.15	J/mol×K	948.63	Joback Method
cpg	775.75	J/mol×K	979.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346604&Units=SI
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

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