L-Valine, N-pentafluorobenzoyl-, pentyl ester

Inchi: InChI=1S/C17H20F5NO3/c1-4-5-6-7-26-17(25)15(8(2)3)23-16(24)9-10(18)12(20)14(22)1
InchiKey: BWCHYXCAWRMRDI-UHFFFAOYSA-N
Formula: C17H20F5NO3
SMILES: CCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 381.34

Physical Properties

Property code	Value	Unit	Source
gf	-1095.86	kJ/mol	Joback Method
hf	-1510.05	kJ/mol	Joback Method
hfus	49.72	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	3.870		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	815.74	K	Joback Method
tc	1004.41	K	Joback Method
tf	518.07	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.44	J/mol×K	815.74	Joback Method
cpg	781.46	J/mol×K	847.19	Joback Method
cpg	793.61	J/mol×K	878.63	Joback Method
cpg	804.89	J/mol×K	910.08	Joback Method
cpg	815.33	J/mol×K	941.52	Joback Method
cpg	824.92	J/mol×K	972.97	Joback Method
cpg	833.68	J/mol×K	1004.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346605&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

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