L-Valine, N-pentafluorobenzoyl-, hexyl ester

Inchi: InChI=1S/C18H22F5NO3/c1-4-5-6-7-8-27-18(26)16(9(2)3)24-17(25)10-11(19)13(21)15(2
InchiKey: METAZXMPMHJCPX-UHFFFAOYSA-N
Formula: C18H22F5NO3
SMILES: CCCCCCOC(=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	-1087.44	kJ/mol	Joback Method
hf	-1530.69	kJ/mol	Joback Method
hfus	52.31	kJ/mol	Joback Method
hvap	78.72	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.260		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	838.62	K	Joback Method
tc	1029.77	K	Joback Method
tf	529.34	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.52	J/mol×K	838.62	Joback Method
cpg	838.96	J/mol×K	870.48	Joback Method
cpg	851.46	J/mol×K	902.34	Joback Method
cpg	863.04	J/mol×K	934.20	Joback Method
cpg	873.71	J/mol×K	966.05	Joback Method
cpg	883.49	J/mol×K	997.91	Joback Method
cpg	892.38	J/mol×K	1029.77	Joback Method

Sources

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=U346607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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