L-Valine, N-pentafluorobenzoyl-, octyl ester

Inchi: InChI=1S/C20H26F5NO3/c1-4-5-6-7-8-9-10-29-20(28)18(11(2)3)26-19(27)12-13(21)15(2
InchiKey: DETTUEPUDKGONU-UHFFFAOYSA-N
Formula: C20H26F5NO3
SMILES: CCCCCCCCOC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 423.42

Physical Properties

Property code	Value	Unit	Source
gf	-1070.60	kJ/mol	Joback Method
hf	-1571.97	kJ/mol	Joback Method
hfus	57.49	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	5.040		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	884.38	K	Joback Method
tc	1082.90	K	Joback Method
tf	551.88	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.11	J/mol×K	884.38	Joback Method
cpg	956.37	J/mol×K	917.47	Joback Method
cpg	969.55	J/mol×K	950.55	Joback Method
cpg	981.67	J/mol×K	983.64	Joback Method
cpg	992.75	J/mol×K	1016.73	Joback Method
cpg	1002.80	J/mol×K	1049.82	Joback Method
cpg	1011.86	J/mol×K	1082.90	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=U346609&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