l-Valine, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C14H22F5NO3/c1-4-5-6-7-8-23-11(21)10(9(2)3)20-12(22)13(15,16)14(17,18)1
InchiKey: QLCUAQBNERQVAA-UHFFFAOYSA-N
Formula: C14H22F5NO3
SMILES: CCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 347.32

Physical Properties

Property code	Value	Unit	Source
gf	-1179.70	kJ/mol	Joback Method
hf	-1644.81	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.448		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	689.06	K	Joback Method
tc	859.18	K	Joback Method
tf	400.08	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.22	J/mol×K	689.06	Joback Method
cpg	711.39	J/mol×K	717.41	Joback Method
cpg	724.76	J/mol×K	745.77	Joback Method
cpg	737.35	J/mol×K	774.12	Joback Method
cpg	749.21	J/mol×K	802.47	Joback Method
cpg	760.36	J/mol×K	830.83	Joback Method
cpg	770.86	J/mol×K	859.18	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=U320881&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