l-Valine, n-pentafluoropropionyl-, ethyl ester

Inchi: InChI=1S/C10H14F5NO3/c1-4-19-7(17)6(5(2)3)16-8(18)9(11,12)10(13,14)15/h5-6H,4H2
InchiKey: NQHFVNYQFLOUKD-UHFFFAOYSA-N
Formula: C10H14F5NO3
SMILES: CCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 291.22

Physical Properties

Property code	Value	Unit	Source
gf	-1213.38	kJ/mol	Joback Method
hf	-1562.25	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.888		Crippen Method
mcvol	179.600	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
tb	597.54	K	Joback Method
tc	768.17	K	Joback Method
tf	355.00	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.65	J/mol×K	597.54	Joback Method
cpg	501.97	J/mol×K	625.98	Joback Method
cpg	513.56	J/mol×K	654.42	Joback Method
cpg	524.47	J/mol×K	682.85	Joback Method
cpg	534.71	J/mol×K	711.29	Joback Method
cpg	544.32	J/mol×K	739.73	Joback Method
cpg	553.32	J/mol×K	768.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320878&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