L-Valine, N-acetyl-

Other names: Valine, N-acetyl-, L-
Acetylvaline
N-Acetyl-L-valine
N-Acetylvaline
Inchi: InChI=1S/C7H13NO3/c1-4(2)6(7(10)11)8-5(3)9/h4,6H,1-3H3,(H,8,9)(H,10,11)/t6-/m0/s1
InchiKey: IHYJTAOFMMMOPX-LURJTMIESA-N
Formula: C7H13NO3
SMILES: CC(=O)NC(C(=O)O)C(C)C
Mol. weight [g/mol]: 159.18
CAS: 96-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-302.09	kJ/mol	Joback Method
hf	-522.29	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	67.01	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.232		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	608.77	K	Joback Method
tc	795.87	K	Joback Method
tf	351.99	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.77	J/mol×K	608.77	Joback Method
cpg	335.59	J/mol×K	639.95	Joback Method
cpg	344.89	J/mol×K	671.14	Joback Method
cpg	353.70	J/mol×K	702.32	Joback Method
cpg	362.02	J/mol×K	733.50	Joback Method

cpg	369.86	J/mol×K	764.68	Joback Method
cpg	377.24	J/mol×K	795.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96811&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume