N-acetyl-N'-methyl-DL-valinamide

Other names: 2-(acetylamino)-N,3-dimethylbutanamide
Inchi: InChI=1S/C8H16N2O2/c1-5(2)7(8(12)9-4)10-6(3)11/h5,7H,1-4H3,(H,9,12)(H,10,11)
InchiKey: CERMWOUCIZTOBO-UHFFFAOYSA-N
Formula: C8H16N2O2
SMILES: CNC(=O)C(NC(C)=O)C(C)C
Mol. weight [g/mol]: 172.23

Physical Properties

Property code	Value	Unit	Source
gf	-67.46	kJ/mol	Joback Method
hf	-337.23	kJ/mol	Joback Method
hfus	37.23	kJ/mol	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
hvap	58.99	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	-0.107		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	589.64	K	Joback Method
tc	786.10	K	Joback Method
tf	355.10	K	Joback Method
tt	496.72	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.33	J/mol×K	589.64	Joback Method
cpg	383.03	J/mol×K	622.38	Joback Method
cpg	395.05	J/mol×K	655.13	Joback Method

cpg	406.41	J/mol×K	687.87	Joback Method
cpg	417.12	J/mol×K	720.61	Joback Method
cpg	427.21	J/mol×K	753.35	Joback Method
cpg	436.69	J/mol×K	786.10	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups:	https://www.doi.org/10.1016/j.jct.2013.12.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume