

2-(Acetylamino)-N-methylethanamide

Other names:	2-acetamido-N-methylacetamide N-acetyl-N'-methylglycinamide N-acetylglycine methylamide acetamide, 2-(acetylamino)-N-methyl-
Inchi:	InChI=1S/C5H10N2O2/c1-4(8)7-3-5(9)6-2/h3H2,1-2H3,(H,6,9)(H,7,8)
InchiKey:	FJMAXCRRCJSCIE-UHFFFAOYSA-N
Formula:	C5H10N2O2
SMILES:	CNC(=O)CNC(C)=O
Mol. weight [g/mol]:	130.15
CAS:	7606-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-87.84	kJ/mol	Joback Method
hf	-264.75	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
hvap	53.09	kJ/mol	Joback Method
log10ws	0.16		Crippen Method
logp	-1.131		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	521.88	K	Joback Method
tc	718.28	K	Joback Method
tf	351.29	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.16	J/mol×K	652.82	Joback Method
cpg	276.75	J/mol×K	685.55	Joback Method

cpg	234.24	J/mol×K	521.88	Joback Method
cpg	243.68	J/mol×K	554.61	Joback Method
cpg	252.63	J/mol×K	587.35	Joback Method
cpg	261.12	J/mol×K	620.08	Joback Method
cpg	283.90	J/mol×K	718.28	Joback Method
cps	177.75	J/mol×K	298.00	NIST Webbook
hsubt	97.80	kJ/mol	355.50	NIST Webbook

Sources

Thermal properties of some small peptides (N-acetyl-amino acids, methionine, and their interactions with nucleic acids)	https://www.doi.org/10.1016/j.jct.2013.12.016
Partial Molar Heat Capacities at Chosen Temperatures in the Range (298.15 to 308.15) K and Partial Molar Volumes at 298.15 K of N-Acetyl-N-methyl-L-alpha,-amino Acid Amides in Aqueous Solution : NIST Webbook.	https://www.doi.org/10.1021/je2012555
Crippen Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7606793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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