

N-Acetyl-dl-alanine methylamide

Other names:	2-(Acetylamino)-N-methylpropanamide 2-(Acetylamino)-N-methylpropanamide (DL) 2-acetamido-N-methylpropanamide N2-acetyl-N-methylalaninamide
Inchi:	InChI=1S/C6H12N2O2/c1-4(6(10)7-3)8-5(2)9/h4H,1-3H3,(H,7,10)(H,8,9)
InchiKey:	VHCVPWSUVMHJLL-UHFFFAOYSA-N
Formula:	C6H12N2O2
SMILES:	CNC(=O)C(C)NC(C)=O
Mol. weight [g/mol]:	144.17
CAS:	34276-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-81.86	kJ/mol	Joback Method
hf	-290.67	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.743		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	544.32	K	Joback Method
tc	742.19	K	Joback Method
tf	347.56	K	Joback Method
tt	411.90	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.87	J/mol×K	544.32	Joback Method

cpg	288.60	J/mol×K	577.30	Joback Method
cpg	298.76	J/mol×K	610.28	Joback Method
cpg	308.38	J/mol×K	643.25	Joback Method
cpg	317.47	J/mol×K	676.23	Joback Method
cpg	326.04	J/mol×K	709.21	Joback Method
cpg	334.10	J/mol×K	742.19	Joback Method
cps	196.47	J/mol×K	298.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34276272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal properties of some small peptides (N-acetyl-amino acids and amides) 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

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
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

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