

N-acetyl-N'-methyl-DL-leucinamide

Other names:	2-(acetylamino)-N,4-dimethylpentanamide
Inchi:	InChI=1S/C9H18N2O2/c1-6(2)5-8(9(13)10-4)11-7(3)12/h6,8H,5H2,1-4H3,(H,10,13)(H,11)
InchiKey:	GFQFFCFJVLJXRY-UHFFFAOYSA-N
Formula:	C9H18N2O2
SMILES:	CNC(=O)C(CC(C)C)NC(C)=O
Mol. weight [g/mol]:	186.26

Physical Properties

Property code	Value	Unit	Source
gf	-59.04	kJ/mol	Joback Method
hf	-357.87	kJ/mol	Joback Method
hfus	27.16	kJ/mol	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
hvap	61.22	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.283		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	612.52	K	Joback Method
tc	806.48	K	Joback Method
tf	366.37	K	Joback Method
tt	432.10	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
vc	0.610	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.88	J/molxK	612.52	Joback Method
cpg	432.27	J/molxK	644.85	Joback Method
cpg	444.94	J/molxK	677.17	Joback Method

cpg	456.92	J/mol×K	709.50	Joback Method
cpg	468.22	J/mol×K	741.83	Joback Method
cpg	478.86	J/mol×K	774.16	Joback Method
cpg	488.87	J/mol×K	806.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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