

N-Acetylnorvaline methylamide

Other names:	2-(acetylamino)-N-methylpentanamide N-Acetylnorvaline-N'-methylamide (DL) N-acetyl-N'-methyl-DL-norvalinamide
Inchi:	InChI=1S/C8H16N2O2/c1-4-5-7(8(12)9-3)10-6(2)11/h7H,4-5H2,1-3H3,(H,9,12)(H,10,11)
InchiKey:	SKSIAIMVWBILBT-UHFFFAOYSA-N
Formula:	C8H16N2O2
SMILES:	CCCC(NC(C)=O)C(=O)NC
Mol. weight [g/mol]:	172.22
CAS:	33067-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-65.02	kJ/mol	Joback Method
hf	-331.95	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	0.037		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	590.08	K	Joback Method
tc	782.80	K	Joback Method
tf	370.10	K	Joback Method
tt	432.29	K	Thermal properties of some small peptides (N-acetyl-amino acid-N'-methylamides) with non-polar side groups
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.91	J/mol×K	590.08	Joback Method
cpg	382.32	J/mol×K	622.20	Joback Method

cpg	394.08	J/mol×K	654.32	Joback Method
cpg	405.21	J/mol×K	686.44	Joback Method
cpg	415.74	J/mol×K	718.56	Joback Method
cpg	425.66	J/mol×K	750.68	Joback Method
cpg	435.02	J/mol×K	782.80	Joback Method
cps	239.69	J/mol×K	298.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal properties of some small peptides (N-acetyl-amino acids, 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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33067468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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