

N-Acetyl-L-alanine amide

Inchi:	InChI=1S/C5H10N2O2/c1-3(5(6)9)7-4(2)8/h3H,1-2H3,(H2,6,9)(H,7,8)
InchiKey:	DVOVBGJJSFSOPZ-UHFFFAOYSA-N
Formula:	C5H10N2O2
SMILES:	CC(=O)NC(C)C(N)=O
Mol. weight [g/mol]:	130.15
CAS:	15962-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-113.22	kJ/mol	Joback Method
hf	-289.71	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hsub	118.10 ± 1.60	kJ/mol	NIST Webbook
hvap	56.91	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	-1.004		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	543.80	K	Joback Method
tc	753.31	K	Joback Method
tf	366.89	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.65	J/molxK	543.80	Joback Method
cpg	284.94	J/molxK	718.39	Joback Method
cpg	277.49	J/molxK	683.47	Joback Method
cpg	269.55	J/molxK	648.56	Joback Method
cpg	261.10	J/molxK	613.64	Joback Method
cpg	252.14	J/molxK	578.72	Joback Method
cpg	291.91	J/molxK	753.31	Joback Method
hfust	21.70	kJ/mol	431.00	NIST Webbook

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hfust	21.70	kJ/mol	431.00	NIST Webbook
hsubt	115.00 ± 3.00	kJ/mol	388.00	NIST Webbook
hsubt	115.00 ± 1.20	kJ/mol	376.00	NIST Webbook
sfust	50.30	J/mol×K	431.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C15962477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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