

N-«alpha»-Acetylglycinamide

Other names:	N-Acetylglycine amide Acetamide, N-(2-amino-2-oxoethyl)- N-Acetylglycinamide 2-acetamidoacetamide
Inchi:	InChI=1S/C4H8N2O2/c1-3(7)6-2-4(5)8/h2H2,1H3,(H2,5,8)(H,6,7)
InchiKey:	WQELDIQOHGAHEM-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	CC(=O)NCC(N)=O
Mol. weight [g/mol]:	114.10
CAS:	2620-63-5

Physical Properties

Property code	Value	Unit	Source
gf	-119.20	kJ/mol	Joback Method
hf	-263.79	kJ/mol	Joback Method
hfus	19.61	kJ/mol	Joback Method
hsub	140.20 ± 2.30	kJ/mol	NIST Webbook
hsub	140.20 ± 2.30	kJ/mol	NIST Webbook
hvap	55.07	kJ/mol	Joback Method
log10ws	0.33		Crippen Method
logp	-1.392		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	521.36	K	Joback Method
tc	729.58	K	Joback Method
tf	370.62	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.29	J/mol×K	521.36	Joback Method
cpg	208.37	J/mol×K	556.06	Joback Method
cpg	216.02	J/mol×K	590.77	Joback Method

cpg	223.24	J/mol×K	625.47	Joback Method
cpg	230.04	J/mol×K	660.18	Joback Method
cpg	236.43	J/mol×K	694.88	Joback Method
cpg	242.42	J/mol×K	729.58	Joback Method
hfust	25.60	kJ/mol	408.20	NIST Webbook
hfust	25.60	kJ/mol	408.20	NIST Webbook
hfust	25.60	kJ/mol	408.20	NIST Webbook
hfust	25.60	kJ/mol	408.20	NIST Webbook
hsubt	123.50 ± 1.70	kJ/mol	376.00	NIST Webbook
hsubt	135.00 ± 3.00	kJ/mol	392.00	NIST Webbook
sfust	62.70	J/mol×K	408.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2620635&Units=SI

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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