Acetamide, N-(aminocarbonyl)-

Other names:	1-Acetylurea
	Acetic acid, ureide
	Acetylcarbamide
	Acetylurea
	Monoacetylurea
	N-Acetylurea
	Urea, acetyl-
Inchi:	InChI=1S/C3H6N2O2/c1-2(6)5-3(4)7/h1H3,(H3,4,5,6,7)
InchiKey:	GKRZNOGGALENQJ-UHFFFAOYSA-N
Formula:	C3H6N2O2
SMILES:	CC(=O)NC(N)=O
Mol. weight [g/mol]:	102.09
CAS:	591-07-1

Physical Properties

Property code	Value	Unit	Source
chs	-1493.30 ± 0.30	kJ/mol	NIST Webbook
gf	-127.62	kJ/mol	Joback Method
hf	-441.70 ± 0.90	kJ/mol	NIST Webbook
hfs	-544.74 ± 0.55	kJ/mol	NIST Webbook
hfus	17.02	kJ/mol	Joback Method
hsub	103.10 ± 0.70	kJ/mol	NIST Webbook
hsub	103.10 ± 0.70	kJ/mol	NIST Webbook
hsub	103.05 ± 0.67	kJ/mol	NIST Webbook
hvap	52.84	kJ/mol	Joback Method
ie	10.30	eV	NIST Webbook
log10ws	-0.90		Aqueous Solubility Prediction Method
logp	-0.799		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method
tb	498.48	K	Joback Method
tc	709.93	K	Joback Method
tf	359.35	K	Joback Method
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.68	J/mol×K	674.69	Joback Method
cpg	160.31	J/mol×K	498.48	Joback Method
cpg	167.11	J/mol×K	533.72	Joback Method
cpg	173.54	J/mol×K	568.96	Joback Method
cpg	179.61	J/mol×K	604.20	Joback Method
cpg	185.32	J/mol×K	639.44	Joback Method
cpg	195.70	J/mol×K	709.93	Joback Method
hsubt	102.40 ± 0.70	kJ/mol	383.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591071&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
vc:	Critical Volume