Urea

Other names:	(NH2)2CO
	Alphadrate
	Aquacare
	Aquadrate
	B-I-K
	Basodexan
	Benural 70
	Bubber shet
	Calmurid
	Carbaderm
	Carbamide
	Carbamimidic acid
	Carbonyl Diamine
	Carbonyldiamide
	Elaqua xx
	Harnstoff
	Hyanit
	Isourea
	Keratinamin
	Mocovina
	NCI-C02119
	NSC 34375
	Nutraplus
	Onychomal
	Pastaron
	Prespersion, 75 urea
	Pseudourea
	Supercel 3000
	UR
	Ultra Mide
	Urea-13C
	Ureaphil
	Ureophil
	Urepearl
	Urevert
	Uroderm
	Varioform II
	carbamoylamine
Inchi:	InChI=1S/CH4N2O/c2-1(3)4/h(H4,2,3,4)
InchiKey:	XSQUKJJJFZCRTK-UHFFFAOYSA-N

Formula: CH4N2O
SMILES: NC(N)=O
Mol. weight [g/mol]: 60.06
CAS: 57-13-6

Physical Properties

Property code	Value	Unit	Source
affp	868.40 ± 2.50	kJ/mol	NIST Webbook
affp	873.50 ± 5.00	kJ/mol	NIST Webbook
affp	873.50 ± 5.00	kJ/mol	NIST Webbook
basg	841.60 ± 5.00	kJ/mol	NIST Webbook
basg	846.10 ± 5.00	kJ/mol	NIST Webbook
basg	838.70 ± 3.00	kJ/mol	NIST Webbook
ep	9.40	J/mol×K	NIST Webbook
ep	-1.90	J/mol×K	NIST Webbook
gf	-38.48	kJ/mol	Joback Method
hf	-235.50 ± 1.20	kJ/mol	NIST Webbook
hfs	-333.30 ± 0.20	kJ/mol	NIST Webbook
hfs	-323.60	kJ/mol	NIST Webbook
hfs	-333.11 ± 0.69	kJ/mol	NIST Webbook
hfs	-333.39 ± 0.17	kJ/mol	NIST Webbook
hfs	-320.20 ± 2.00	kJ/mol	NIST Webbook
hfus	10.34	kJ/mol	Joback Method
hsub	87.65 ± 0.88	kJ/mol	NIST Webbook
hsub	95.50 ± 0.30	kJ/mol	NIST Webbook
hsub	98.60	kJ/mol	NIST Webbook
hvap	45.85	kJ/mol	Joback Method
ie	10.27 ± 0.05	eV	NIST Webbook
ie	10.28	eV	NIST Webbook
ie	10.33	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
log10ws	0.96		Aqueous Solubility Prediction Method
log10ws	0.96		Estimated Solubility Method
logp	-0.976		Crippen Method
mcvol	46.480	ml/mol	McGowan Method
pc	7735.33	kPa	Joback Method
ss	105.40	J/mol×K	NIST Webbook

ss	104.26	J/mol×K	NIST Webbook
ss	104.93	J/mol×K	NIST Webbook
ss	172.00	J/mol×K	NIST Webbook
tb	421.21	K	Joback Method
tc	638.13	K	Joback Method
tf	406.20 ± 0.10	K	NIST Webbook
tf	406.00 ± 3.00	K	NIST Webbook
tf	406.15 ± 1.50	K	NIST Webbook
tf	405.15 ± 1.50	K	NIST Webbook
tf	405.80 ± 0.50	K	NIST Webbook
tf	407.00	K	Aqueous Solubility Prediction Method
tf	410.00 ± 1.50	K	NIST Webbook
tf	406.50 ± 0.50	K	NIST Webbook
tf	405.40 ± 0.80	K	NIST Webbook
tt	407.90 ± 0.20	K	NIST Webbook
tt	408.00 ± 0.00	K	NIST Webbook
tt	405.80 ± 0.20	K	NIST Webbook
tt	405.80 ± 0.10	K	NIST Webbook
vc	0.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.80	J/mol×K	421.21	Joback Method
cpg	91.98	J/mol×K	457.36	Joback Method
cpg	95.96	J/mol×K	493.52	Joback Method
cpg	99.73	J/mol×K	529.67	Joback Method
cpg	103.30	J/mol×K	565.82	Joback Method
cpg	106.68	J/mol×K	601.98	Joback Method
cpg	109.86	J/mol×K	638.13	Joback Method
cps	115.50	J/mol×K	298.00	NIST Webbook
cps	94.00	J/mol×K	304.70	NIST Webbook
cps	93.08	J/mol×K	298.15	NIST Webbook
cps	90.00	J/mol×K	298.15	NIST Webbook
cps	93.14	J/mol×K	298.15	NIST Webbook
cps	92.79	J/mol×K	298.15	NIST Webbook
cps	93.64	J/mol×K	298.00	NIST Webbook
cps	68.60	J/mol×K	293.00	NIST Webbook
hfust	14.79	kJ/mol	406.50	NIST Webbook
hfust	13.90	kJ/mol	405.80	NIST Webbook

hfust	14.50	kJ/mol	406.00	NIST Webbook
hfust	13.61	kJ/mol	405.80	NIST Webbook
hfust	14.60	kJ/mol	407.20	NIST Webbook
hfust	13.60	kJ/mol	405.20	NIST Webbook
hfust	14.60	kJ/mol	406.70	NIST Webbook
hfust	15.03	kJ/mol	407.90	NIST Webbook
hfust	12.93	kJ/mol	408.10	NIST Webbook
hfust	13.90	kJ/mol	405.80	NIST Webbook
hsubt	88.20	kJ/mol	357.00	NIST Webbook
hsubt	95.10 ± 2.20	kJ/mol	366.00	NIST Webbook
hsubt	94.60 ± 0.50	kJ/mol	350.00	NIST Webbook
hsubt	97.60 ± 1.00	kJ/mol	354.00	NIST Webbook
hsubt	90.90	kJ/mol	381.00	NIST Webbook
hsubt	87.70	kJ/mol	356.50	NIST Webbook
hsubt	96.90	kJ/mol	350.00	NIST Webbook
hsubt	95.40	kJ/mol	361.00	NIST Webbook
hsubt	87.90 ± 2.10	kJ/mol	356.50	NIST Webbook
hsubt	94.60 ± 2.20	kJ/mol	366.00	NIST Webbook
psub	0.02	kPa	399.00	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea
psub	1.00e-03	kPa	363.40	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea

psub	0.02	kPa	402.00	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea	
psub	1.89e-03	kPa	371.20	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea	
psub	2.46e-03	kPa	374.30	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea	
psub	2.96e-03	kPa	376.50	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea	

psub	3.80e-03	kPa	379.50	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea
psub	6.27e-03	kPa	386.30	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea
psub	0.01	kPa	393.20	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea
psub	6.40e-04	kPa	358.30	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea

psub	1.51e-03	kPa	368.40	Measurement and Prediction of Thermochemical Properties: Improved Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea
sfust	33.54	J/mol×K	405.80	NIST Webbook
sfust	36.40	J/mol×K	406.50	NIST Webbook
sfust	34.25	J/mol×K	405.80	NIST Webbook
sfust	35.70	J/mol×K	406.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.20584e+01
Coeff. B	-1.05730e+04
Coeff. C	6.10000e-01
Temperature range (K), min.	340.65
Temperature range (K), max.	368.05

Sources

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Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ep:	Protonation entropy at 298K
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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume