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
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	846.10 ± 5.00	kJ/mol	NIST Webbook
basg	841.60 ± 5.00	kJ/mol	NIST Webbook
basg	838.70 ± 3.00	kJ/mol	NIST Webbook
ep	-1.90	J/mol×K	NIST Webbook
ep	9.40	J/mol×K	NIST Webbook
gf	-38.48	kJ/mol	Joback Method
hf	-235.50 ± 1.20	kJ/mol	NIST Webbook
hfs	-333.11 ± 0.69	kJ/mol	NIST Webbook
hfs	-333.39 ± 0.17	kJ/mol	NIST Webbook
hfs	-333.30 ± 0.20	kJ/mol	NIST Webbook
hfs	-323.60	kJ/mol	NIST Webbook
hfs	-320.20 ± 2.00	kJ/mol	NIST Webbook
hfus	10.34	kJ/mol	Joback Method
hsub	95.50 ± 0.30	kJ/mol	NIST Webbook
hsub	98.60	kJ/mol	NIST Webbook
hsub	87.65 ± 0.88	kJ/mol	NIST Webbook
hvap	45.85	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	10.33	eV	NIST Webbook
ie	10.27 ± 0.05	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	10.28	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	104.93	J/mol×K	NIST Webbook
ss	105.40	J/mol×K	NIST Webbook

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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:	https://www.doi.org/10.1021/je050230z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1456
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
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