Urea, N,N'-dimethyl-

Other names:	(CH3NH)2CO
	1,1'-Dimethylurea
	1,3-dimethylurea
	DMU
	N,N'-Dimethylharnstoff
	N,N'-dimethylurea
	NSC 14910
	Symmetric dimethylurea
	sym-Dimethylurea
	urea, 1,3-dimethyl-
Inchi:	InChI=1S/C3H8N2O/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)
InchiKey:	MGJKQDOBUOMPEZ-UHFFFAOYSA-N
Formula:	C3H8N2O
SMILES:	CNC(=O)NC
Mol. weight [g/mol]:	88.11
CAS:	96-31-1

Physical Properties

Property code	Value	Unit	Source
affp	903.30	kJ/mol	NIST Webbook
basg	873.50	kJ/mol	NIST Webbook
chs	-2011.70 ± 2.80	kJ/mol	NIST Webbook
chs	-2010.20 ± 1.10	kJ/mol	NIST Webbook
gf	24.24	kJ/mol	Joback Method
hf	-221.60 ± 1.60	kJ/mol	NIST Webbook
hfs	-312.10 ± 2.80	kJ/mol	NIST Webbook
hfs	-313.70 ± 1.20	kJ/mol	NIST Webbook
hfus	15.32	kJ/mol	Joback Method
hsub	89.30 ± 0.40	kJ/mol	NIST Webbook
hvap	41.89	kJ/mol	Joback Method
ie	9.23	eV	NIST Webbook
ie	9.42 ± 0.05	eV	NIST Webbook
log10ws	-0.21		Crippen Method
logp	-0.455		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
tb	542.20	K	NIST Webbook

tc	612.72	K	Joback Method
tf	379.50 ± 0.20	K	NIST Webbook
tf	377.50 ± 0.50	K	NIST Webbook
tf	376.35	K	Measurement and correlation of solubility and solution thermodynamics of 1,3-dimethylurea in different solvents from T = (288.15 to 328.15) K
tf	379.90 ± 0.10	K	NIST Webbook
tt	376.35	K	Thermodynamics of 1,3-dimethylurea in eight alcohols
tt	371.00 ± 0.00	K	NIST Webbook
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.78	J/mol×K	580.97	Joback Method
cpg	172.37	J/mol×K	549.23	Joback Method
cpg	165.65	J/mol×K	517.48	Joback Method
cpg	158.59	J/mol×K	485.74	Joback Method
cpg	151.21	J/mol×K	453.99	Joback Method
cpg	184.88	J/mol×K	612.72	Joback Method
cpg	143.48	J/mol×K	422.25	Joback Method
hfust	13.62	kJ/mol	379.50	NIST Webbook
hsubt	87.50 ± 1.00	kJ/mol	347.00	NIST Webbook
hsubt	86.60 ± 0.50	kJ/mol	350.00	NIST Webbook
hsubt	92.10 ± 1.00	kJ/mol	354.00	NIST Webbook
hsubt	87.20 ± 0.60	kJ/mol	344.50	NIST Webbook
hsubt	87.60 ± 1.00	kJ/mol	347.00	NIST Webbook
psub	7.38e-03	kPa	351.40	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	9.66e-03	kPa	354.60	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	357.70	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	5.10e-04	kPa	322.90	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	3.68e-03	kPa	343.20	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	2.42e-03	kPa	339.00	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	1.75e-03	kPa	335.00	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	1.19e-03	kPa	330.90	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	7.70e-04	kPa	326.90	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	1.90e-04	kPa	313.30	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	5.32e-03	kPa	347.30	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
sfust	35.90	J/mol×K	379.50	NIST Webbook

Sources

Density and Viscosity of Aqueous Solutions of 1,3-Dimethylurea from (288.15 to 333.15) K:	https://www.doi.org/10.1021/je900444h
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Densimetric and ultrasonic characterization of urea and its derivatives in water:	https://www.doi.org/10.1016/j.jct.2012.11.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96311&Units=SI
Apparent molar volumes and apparent molar heat capacities of aqueous urea, 1,1-dimethylurea, and 1,3-dimethylurea at temperatures from (278.15 to 348.15) K and at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2005.10.017
Apparent Molar Volumes and Expansibilities of Thiourea, 1,3-Dimethylthiourea in Water at Temperatures from T = (278.15 to 318.15) K and Atmospheric Pressure:	https://www.doi.org/10.1021/je301203z
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermal Expansion and Structure of 1,3-Dimethylurea, Tetramethylurea, and Tetrabutylammonium Bromide in Aqueous Solutions:	https://www.doi.org/10.1021/je900164a
Volumetric and solution thermodynamics of urea and 1,3-dimethylurea in different solvents from T = (288.15 to 328.15) K:	https://www.doi.org/10.1016/j.jct.2015.12.032
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density Measurements:	
Thermodynamics of 1,3-dimethylurea in eight alcohols:	https://www.doi.org/10.1021/acs.jced.5b00882
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume