Urea, N,N-dimethyl-

Other names:	(CH3)2NCONH2
	1,1-dimethylurea
	Asym-Dimethylurea
	N,N-dimethylcarbamide
	N,N-dimethylurea
	Urea, 1,1-dimethyl-
Inchi:	InChI=1S/C3H8N2O/c1-5(2)3(4)6/h1-2H3,(H2,4,6)
InchiKey:	YBBLOADPFWKNGS-UHFFFAOYSA-N
Formula:	C3H8N2O
SMILES:	CN(C)C(N)=O
Mol. weight [g/mol]:	88.11
CAS:	598-94-7

Physical Properties

Property code	Value	Unit	Source
chs	-2004.80 ± 0.53	kJ/mol	NIST Webbook
gf	22.69	kJ/mol	Joback Method
hf	-220.00 ± 1.10	kJ/mol	NIST Webbook
hfs	-319.06 ± 0.68	kJ/mol	NIST Webbook
hfus	13.34	kJ/mol	Joback Method
hsub	93.50 ± 0.30	kJ/mol	NIST Webbook
hvap	41.70	kJ/mol	Joback Method
ie	9.10 ± 0.05	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	0.16		Crippen Method
logp	-0.373		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
tb	406.88	K	Joback Method
tc	601.80	K	Joback Method
tf	454.00 ± 0.50	K	NIST Webbook
tf	455.20 ± 0.10	K	NIST Webbook
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.70	J/mol×K	569.31	Joback Method
cpg	143.54	J/mol×K	406.88	Joback Method
cpg	151.56	J/mol×K	439.37	Joback Method
cpg	159.17	J/mol×K	471.85	Joback Method
cpg	166.39	J/mol×K	504.34	Joback Method
cpg	173.23	J/mol×K	536.83	Joback Method
cpg	185.82	J/mol×K	601.80	Joback Method
hfust	29.11	kJ/mol	454.00	NIST Webbook
hfust	29.61	kJ/mol	454.00	NIST Webbook
hsubt	92.50 ± 1.30	kJ/mol	347.50	NIST Webbook
hsubt	94.70 ± 1.40	kJ/mol	347.50	NIST Webbook
hsubt	94.70 ± 1.40	kJ/mol	347.50	NIST Webbook
hsubt	93.30 ± 0.50	kJ/mol	350.00	NIST Webbook
hsubt	99.10 ± 0.90	kJ/mol	353.00	NIST Webbook
psub	0.20	kPa	398.30	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	3.14e-03	kPa	346.30	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	7.53e-03	kPa	356.10	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	362.20	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	0.02	kPa	365.20	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	0.02	kPa	368.10	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	0.03	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	0.03	kPa	374.20	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	0.04	kPa	377.20	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	0.05	kPa	380.20	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	0.07	kPa	383.30	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	0.09	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	0.11	kPa	389.30	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	0.13	kPa	392.20	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	0.16	kPa	395.20	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
sfust	65.20	J/mol×K	454.00	NIST Webbook

Sources

Apparent molar volumes and apparent molar heat capacities of aqueous urea, 1,1-dimethylurea, and	https://www.doi.org/10.1016/j.jct.2005.10.017
Hydration of urea and its derivatives -	https://www.doi.org/10.1016/j.jct.2014.07.012
Volumetric and compressibility	
1,3-dimethylurea at temperatures from	https://www.doi.org/10.1021/je050230z
Measurement and Prediction of	
0.10 to 348.15) K and at the pressure	
Thermochemical Properties: Improved	https://en.wikipedia.org/wiki/Joback_method
0.10 MPa.	
Increments for the Estimation of	
Joback Method:	
Enthalpies of Sublimation and	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	
Standard Enthalpies of Formation of	
Alkyl Derivatives of Urea:	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
vc:	Critical Volume