Urea, methyl-

Other names:	1-Methylurea
	CH3NHCONH2
	Methylmocovina
	Methylurea
	Monomethylurea
	N-Methylurea
	methyl carbamide
	urea, monomethyl-
Inchi:	InChI=1S/C2H6N2O/c1-4-2(3)5/h1H3,(H3,3,4,5)
InchiKey:	XGEGHDBEHXKFPX-UHFFFAOYSA-N
Formula:	C2H6N2O
SMILES:	CNC(N)=O
Mol. weight [g/mol]:	74.08
CAS:	598-50-5

Physical Properties

Property code	Value	Unit	Source
chs	-1316.80 ± 1.40	kJ/mol	NIST Webbook
chs	-1311.74 ± 0.69	kJ/mol	NIST Webbook
gf	-7.12	kJ/mol	Joback Method
hf	-233.50 ± 1.00	kJ/mol	NIST Webbook
hf	-235.68 ± 0.85	kJ/mol	NIST Webbook
hfs	-327.80 ± 1.40	kJ/mol	NIST Webbook
hfs	-332.78 ± 0.75	kJ/mol	NIST Webbook
hfus	12.74	kJ/mol	Measurement of enthalpy curves of phase change materials via DSC and T-History: When are both methods needed to estimate the behaviour of the bulk material in applications?
hsub	97.10 ± 0.40	kJ/mol	NIST Webbook
hsub	95.50 ± 0.50	kJ/mol	NIST Webbook
hsub	97.10 ± 0.40	kJ/mol	NIST Webbook
hvap	43.87	kJ/mol	Joback Method
ie	9.73 ± 0.05	eV	NIST Webbook
ie	9.66	eV	NIST Webbook

log10ws	1.13		Aqueous Solubility Prediction Method
logp	-0.715		Crippen Method
mcvol	60.570	ml/mol	McGowan Method
pc	6132.23	kPa	Joback Method
ss	138.02	J/mol×K	NIST Webbook
tb	421.73	K	Joback Method
tc	624.80	K	Joback Method
tf	375.30 ± 0.10	K	NIST Webbook
tf	373.80 ± 0.50	K	NIST Webbook
tt	378.00 ± 0.00	K	NIST Webbook
tt	375.00 ± 0.20	K	NIST Webbook
vc	0.217	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.61	J/mol×K	421.73	Joback Method
cpg	127.47	J/mol×K	489.42	Joback Method
cpg	132.99	J/mol×K	523.27	Joback Method
cpg	138.23	J/mol×K	557.11	Joback Method
cpg	143.20	J/mol×K	590.96	Joback Method
cpg	147.92	J/mol×K	624.80	Joback Method
cpg	121.68	J/mol×K	455.58	Joback Method
cps	114.74	J/mol×K	298.15	NIST Webbook
hfust	15.75	kJ/mol	373.80	NIST Webbook
hfust	14.06	kJ/mol	378.10	NIST Webbook
hfust	16.60	kJ/mol	375.00	NIST Webbook
hfust	12.50	kJ/mol	372.00	NIST Webbook
hsubt	94.40 ± 0.84	kJ/mol	343.00	NIST Webbook
hsubt	99.30 ± 0.70	kJ/mol	337.00	NIST Webbook
hsubt	87.30	kJ/mol	348.00	NIST Webbook
hsubt	94.38 ± 0.85	kJ/mol	343.00	NIST Webbook
hsubt	94.40 ± 0.80	kJ/mol	350.00	NIST Webbook
hsubt	93.30 ± 1.20	kJ/mol	355.00	NIST Webbook
hsubt	96.80 ± 1.20	kJ/mol	346.50	NIST Webbook
hsubt	96.90 ± 1.20	kJ/mol	346.50	NIST Webbook
hsubt	94.90 ± 0.60	kJ/mol	337.00	NIST Webbook
hsubt	95.73	kJ/mol	343.00	NIST Webbook

psub	1.92e-03	kPa	349.20	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	8.15e-03	kPa	365.70	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	8.03e-03	kPa	365.70	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	6.12e-03	kPa	362.70	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	3.56e-03	kPa	356.20	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	2.52e-03	kPa	352.20	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	1.40e-03	kPa	346.10	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	1.00e-03	kPa	342.70	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	6.40e-04	kPa	338.10	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	4.00e-04	kPa	333.10	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	4.74e-03	kPa	359.60	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
sfust	42.10	J/mol×K	373.80	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
Densimetric and ultrasonic characterization of urea and its derivatives in water:	https://www.doi.org/10.1016/j.jct.2012.11.007
Measurement of enthalpy curves of phase change materials via DSC and T-History: Which are both methods needed to estimate the behaviour of the bulk material in applications?:	https://www.doi.org/10.1016/j.tca.2014.09.022
Method for Melting Point:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598505&Units=SI
Solubility and thermodynamic properties of NH3 in choline chloride-based deep eutectic solvents:	https://www.doi.org/10.1016/j.jct.2019.01.031

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
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