Urea, tetramethyl-

Other names:	((CH3)2N)2CO
	1,1,3,3-Tetramethylurea
	N,N,N',N'-Tetramethylurea
	NSC 91488
	TMU
	Temur
	Tetramethylurea
	Tetramethyluree
	Urea, 1,1,3,3-tetramethyl-
	Urea, N,N,N',N'-tetramethyl-
	urea, tetramethyl
Inchi:	InChI=1S/C5H12N2O/c1-6(2)5(8)7(3)4/h1-4H3
InchiKey:	AVQQQNCBBIEMEU-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CN(C)C(=O)N(C)C
Mol. weight [g/mol]:	116.16
CAS:	632-22-4

Physical Properties

Property code	Value	Unit	Source
affp	930.60	kJ/mol	NIST Webbook
basg	899.60	kJ/mol	NIST Webbook
chl	-3420.36 ± 0.81	kJ/mol	NIST Webbook
gf	83.86	kJ/mol	Joback Method
hf	-205.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-262.20 ± 1.10	kJ/mol	NIST Webbook
hfus	16.35	kJ/mol	Joback Method
hvap	56.60 ± 0.80	kJ/mol	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.74 ± 0.05	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
log10ws	0.94		Aqueous Solubility Prediction Method
log10ws	0.94		Estimated Solubility Method
logp	0.230		Crippen Method
mcvol	102.840	ml/mol	McGowan Method

pc	3722.56	kPa	Joback Method
tb	449.70	K	NIST Webbook
tc	567.86	K	Joback Method
tf	272.05	K	Aqueous Solubility Prediction Method
tf	272.20 ± 0.10	K	NIST Webbook
tf	272.00 ± 0.10	K	NIST Webbook
tt	270.48 ± 0.02	K	NIST Webbook
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.33	J/mol×K	567.86	Joback Method
cpg	237.32	J/mol×K	509.42	Joback Method
cpg	227.61	J/mol×K	480.21	Joback Method
cpg	217.40	J/mol×K	450.99	Joback Method
cpg	206.67	J/mol×K	421.77	Joback Method
cpg	195.42	J/mol×K	392.55	Joback Method
cpg	246.56	J/mol×K	538.64	Joback Method
cpl	241.20	J/mol×K	320.00	NIST Webbook
hfust	13.40	kJ/mol	272.20	NIST Webbook
hfust	13.40	kJ/mol	272.20	NIST Webbook
hfust	13.40	kJ/mol	272.20	NIST Webbook
hfust	14.00	kJ/mol	272.10	NIST Webbook
hfust	13.40	kJ/mol	272.20	NIST Webbook
hvapt	52.20	kJ/mol	385.00	NIST Webbook
hvapt	41.70	kJ/mol	385.00	NIST Webbook
rhol	962.04	kg/m3	298.15	Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 318.15 K
rhol	971.20	kg/m3	288.15	Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 318.15 K

rhol	943.62	kg/m3	318.15	Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure	
rhol	952.85	kg/m3	308.15	Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure	
rhol	962.05	kg/m3	298.15	Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure	

rhol	971.22	kg/m3	288.15	Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure
rhol	967.00	kg/m3	293.15	Investigation of the Solubilities of Carbon Dioxide in Some Low Volatile Solvents and Their Thermodynamic Properties
rhol	943.62	kg/m3	318.15	Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 318.15 K
rhol	952.84	kg/m3	308.15	Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 318.15 K
rhol	980.34	kg/m3	278.15	Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 318.15 K

rhol	934.38	kg/m3	328.15	Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 K and 328.15 K: A comparative analysis	
rhol	943.65	kg/m3	318.15	Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 K and 328.15 K: A comparative analysis	
rhol	952.88	kg/m3	308.15	Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 K and 328.15 K: A comparative analysis	
rhol	962.07	kg/m3	298.15	Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 K and 328.15 K: A comparative analysis	

rhol	934.35	kg/m3	328.15	Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure	
rhol	971.23	kg/m3	288.15	Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 K and 328.15 K: A comparative analysis	
sfust	49.20	J/mol×K	272.20	NIST Webbook	
sfust	49.20	J/mol×K	272.20	NIST Webbook	
speedsl	1374.53	m/s	303.15	Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl	
speedsl	1393.92	m/s	298.15	Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl	
speedsl	1413.44	m/s	293.15	Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl	

speedsl	1397.60	m/s	298.15	Volumetric and compressibility properties of liquid water as a solute in glycolic, propylene carbonate, and tetramethylurea solutions at T = 298.15 K
speedsl	1355.31	m/s	308.15	Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl
speedsl	1432.53	m/s	288.15	Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.20526e+01
Coeff. B	-3.16454e+03
Coeff. C	-6.47090e+01
Temperature range (K), min.	293.85
Temperature range (K), max.	534.14

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Volume-related interaction parameters for dilute solutions of tetramethylurea in normal and heavy water between 278.15 K and 338.15 K: https://www.doi.org/10.1016/j.tca.2009.12.008

Enthalpy-related interaction parameters in normal and heavy water between 278.15 K and 338.15 K: https://www.doi.org/10.1016/j.tca.2011.05.019

Investigation of the Solubilities of Carbon Dioxide in Some Low-Volatile Solvents and Their Thermodynamic Properties: https://www.doi.org/10.1021/acs.jced.5b00893

Cyclic derivatives at 298.15 K: **Aqueous solubility prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632224&Units=SI
Solubility and thermodynamic properties of SO2 in three low volatile urea derivatives:	https://www.doi.org/10.1016/j.jct.2016.05.004
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densimetric and ultrasonic characterization of urea and its derivatives in water:	https://www.doi.org/10.1016/j.jct.2012.11.007
Solutions of Urea and Tetramethylurea in Formamide and Water: A Comparative Analysis of Volume Characteristics and Solute-Solute Interaction Parameters at Temperatures from 288.15 to 328.15 K and Ambient Pressure:	https://www.doi.org/10.1021/acs.jced.9b00794
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Volumetric and compressibility properties of liquid water as a solute in glycols, propylene carbonate, and tetramethylurea solutions at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2007.05.010
Estimated Solubility:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Volume-related solvation and pair interaction parameters for dilute solutions of urea and tetramethylurea in ethylene glycol between 288.15 and 328.15 K: A comparative analysis:	https://www.doi.org/10.1016/j.jct.2019.04.009
Thermal Expansion and Structure of 1,3-Dimethylurea, Tetramethylurea, and Their Mixtures with Water	https://www.doi.org/10.1021/je900164a
Effect of temperature and ionic strength on volumetric and acoustic properties of urea alkyl derivatives in aqueous NaCl:	https://www.doi.org/10.1016/j.jct.2015.07.002
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density measurements:	

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
sfust:	Entropy of fusion at a given temperature
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume