Urea, N,N'-diethyl-

Other names:	1,3-diethylurea
	N,N'-diethylurea
	sym-Diethylurea
	sym-N,N'-Diethylurea
	urea, 1,3-diethyl-
Inchi:	InChI=1S/C5H12N2O/c1-3-6-5(8)7-4-2/h3-4H2,1-2H3,(H2,6,7,8)
InchiKey:	ZWAVGZYKJNOTPX-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CCNC(=O)NCC
Mol. weight [g/mol]:	116.16
CAS:	623-76-7

Physical Properties

Property code	Value	Unit	Source
chs	-3302.80 ± 1.70	kJ/mol	NIST Webbook
gf	41.08	kJ/mol	Joback Method
hf	-282.90 ± 2.10	kJ/mol	NIST Webbook
hfs	-379.80 ± 1.80	kJ/mol	NIST Webbook
hfus	20.50	kJ/mol	Joback Method
hsub	95.40 ± 0.30	kJ/mol	NIST Webbook
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.325		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	536.20	K	NIST Webbook
tc	654.81	K	Joback Method
tf	383.40 ± 0.50	K	NIST Webbook
tt	385.00 ± 0.00	K	NIST Webbook
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	249.64	J/mol×K	561.41	Joback Method
cpg	220.22	J/mol×K	468.01	Joback Method
cpg	230.48	J/mol×K	499.14	Joback Method
cpg	240.29	J/mol×K	530.28	Joback Method
cpg	275.13	J/mol×K	654.81	Joback Method
cpg	267.05	J/mol×K	623.68	Joback Method
cpg	258.56	J/mol×K	592.54	Joback Method
hfust	12.46	kJ/mol	383.40	NIST Webbook
hfust	12.46	kJ/mol	383.40	NIST Webbook
hsubt	96.80 ± 0.90	kJ/mol	350.00	NIST Webbook
hsubt	91.80 ± 0.90	kJ/mol	353.50	NIST Webbook
hsubt	92.30 ± 0.90	kJ/mol	353.50	NIST Webbook
hsubt	95.60 ± 0.60	kJ/mol	350.00	NIST Webbook
hsubt	96.90 ± 0.90	kJ/mol	354.00	NIST Webbook
psub	0.04	kPa	379.20	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	376.20	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	374.60	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	0.03	kPa	373.20	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	370.10	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	0.02	kPa	367.20	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	0.01	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	0.01	kPa	364.20	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	0.01	kPa	361.20	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	8.50e-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	
psub	7.83e-03	kPa	358.20	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	6.17e-03	kPa	355.20	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	4.76e-03	kPa	352.30	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	3.53e-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	2.70e-03	kPa	346.20	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	2.05e-03	kPa	343.10	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
sfust	32.50	J/mol×K	383.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densimetric and ultrasonic characterization of urea and its derivatives in water:	https://www.doi.org/10.1016/j.jct.2012.11.007
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
McGowan-Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623767&Units=SI

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
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