Urea, butyl-

Other names:	1-butylurea
	N-butylurea
	N-n-Butylurea
	NCI-C02131
	butyl urea
	butylurea
	monobutylurea
	urea, N-butyl-
	urea, monobutyl-
Inchi:	InChI=1S/C5H12N2O/c1-2-3-4-7-5(6)8/h2-4H2,1H3,(H3,6,7,8)
InchiKey:	CNWSQCLBDWYLAN-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CCCCNC(N)=O
Mol. weight [g/mol]:	116.16
CAS:	592-31-4

Physical Properties

Property code	Value	Unit	Source
chs	-3263.10 ± 3.20	kJ/mol	NIST Webbook
gf	18.14	kJ/mol	Joback Method
hf	-313.60 ± 4.20	kJ/mol	NIST Webbook
hfs	-419.50 ± 3.30	kJ/mol	NIST Webbook
hfus	20.60	kJ/mol	Joback Method
hsub	105.80 ± 0.70	kJ/mol	NIST Webbook
hvap	50.55	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.455		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	490.37	K	Joback Method
tc	686.34	K	Joback Method
tf	369.30 ± 0.50	K	NIST Webbook
tt	360.00 ± 0.00	K	NIST Webbook
tt	370.00 ± 0.30	K	NIST Webbook
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.63	J/mol×K	490.37	Joback Method
cpg	239.75	J/mol×K	523.03	Joback Method
cpg	249.39	J/mol×K	555.69	Joback Method
cpg	258.56	J/mol×K	588.36	Joback Method
cpg	267.27	J/mol×K	621.02	Joback Method
cpg	275.54	J/mol×K	653.68	Joback Method
cpg	283.38	J/mol×K	686.34	Joback Method
hfust	10.80	kJ/mol	365.40	NIST Webbook
hfust	14.55	kJ/mol	369.30	NIST Webbook
hfust	15.70	kJ/mol	370.00	NIST Webbook
hfust	14.55	kJ/mol	369.30	NIST Webbook
hfust	7.02	kJ/mol	313.10	NIST Webbook
hfust	0.88	kJ/mol	344.90	NIST Webbook
hfust	14.55	kJ/mol	369.30	NIST Webbook
hsubt	102.70 ± 2.80	kJ/mol	351.50	NIST Webbook
hsubt	103.00 ± 2.80	kJ/mol	351.50	NIST Webbook
hsubt	105.90 ± 2.60	kJ/mol	354.00	NIST Webbook
hsubt	101.10 ± 0.40	kJ/mol	350.00	NIST Webbook
psub	4.30e-04	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	5.90e-04	kPa	349.50	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	8.10e-04	kPa	352.50	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	8.00e-04	kPa	352.50	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	1.20e-03	kPa	356.50	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	1.69e-03	kPa	359.90	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	2.21e-03	kPa	363.00	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	2.20e-03	kPa	363.10	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	2.57e-03	kPa	364.90	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	3.27e-03	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
sfust	39.40	J/mol×K	369.30	NIST Webbook
sfust	22.42	J/mol×K	313.10	NIST Webbook
sfust	2.55	J/mol×K	344.90	NIST Webbook
sfust	39.40	J/mol×K	369.30	NIST Webbook

Sources

Densimetric and ultrasonic characterization of urea and its derivatives in water:	https://www.doi.org/10.1016/j.jct.2012.11.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hydration of urea and its derivatives - Volumetric and compressibility studies:	https://www.doi.org/10.1016/j.jct.2014.07.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C592314&Units=SI
Effect of temperature and ionic strength on volumetric and acoustic properties of solutions of urea alkyl derivatives in aqueous NaCl:	https://www.doi.org/10.1016/j.jct.2015.07.002
Measurement and Prediction of Thermochemical Properties. Improved McGowan Method:	https://www.doi.org/10.1021/je050230z
Improvements for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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