Urea, (1,1-dimethylethyl)-

Other names:	(1,1-dimethylethyl)urea
	N-(1,1-dimethylethyl)urea
	N-tert-butylurea
	Urea, tert-butyl-
	mono-tert-butylurea
	tert-butylurea
	urea, 1,1-dimethylethyl-
	urea, mono-tert-butyl-
Inchi:	InChI=1S/C5H12N2O/c1-5(2,3)7-4(6)8/h1-3H3,(H3,6,7,8)
InchiKey:	JLEHSYHLHLHPAL-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CC(C)(C)NC(N)=O
Mol. weight [g/mol]:	116.16
CAS:	1118-12-3

Physical Properties

Property code	Value	Unit	Source
chs	-3267.80 ± 0.53	kJ/mol	NIST Webbook
gf	20.98	kJ/mol	Joback Method
hf	-314.00 ± 1.50	kJ/mol	NIST Webbook
hfs	-414.73 ± 0.87	kJ/mol	NIST Webbook
hfus	13.19	kJ/mol	Joback Method
hsub	98.20 ± 0.40	kJ/mol	NIST Webbook
hvap	49.25	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.453		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	487.14	K	Joback Method
tc	695.87	K	Joback Method
tf	449.80 ± 0.70	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.72	J/mol×K	695.87	Joback Method
cpg	244.05	J/mol×K	521.93	Joback Method
cpg	254.43	J/mol×K	556.72	Joback Method
cpg	264.15	J/mol×K	591.50	Joback Method
cpg	273.25	J/mol×K	626.29	Joback Method
cpg	281.76	J/mol×K	661.08	Joback Method
cpg	232.97	J/mol×K	487.14	Joback Method
hfust	33.13	kJ/mol	449.80	NIST Webbook
hfust	33.13	kJ/mol	449.80	NIST Webbook
hfust	0.10	kJ/mol	249.00	NIST Webbook
hfust	33.13	kJ/mol	449.80	NIST Webbook
hsubt	97.60 ± 0.80	kJ/mol	352.50	NIST Webbook
hsubt	97.70 ± 0.80	kJ/mol	352.50	NIST Webbook
hsubt	94.40 ± 0.90	kJ/mol	350.00	NIST Webbook
hsubt	100.70 ± 1.20	kJ/mol	354.00	NIST Webbook
hsubt	101.60 ± 0.70	kJ/mol	379.00	NIST Webbook
psub	1.04e-03	kPa	348.20	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	5.10e-04	kPa	340.30	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	2.70e-04	kPa	335.30	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	2.35e-03	kPa	357.00	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	3.15e-03	kPa	360.20	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	4.19e-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	5.23e-03	kPa	366.00	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	7.02e-03	kPa	369.10	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	8.74e-03	kPa	372.20	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	376.10	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	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	0.02	kPa	382.20	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	385.20	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	388.20	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	391.20	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	394.20	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	0.06	kPa	397.20	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	73.60	J/mol×K	449.80	NIST Webbook
sfust	0.41	J/mol×K	249.00	NIST Webbook
sfust	73.65	J/mol×K	449.80	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1118123&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
vc:	Critical Volume