Urea, propyl-

Other names:	1-Propylurea
	N-propylurea
	propylurea
Inchi:	InChI=1S/C4H10N2O/c1-2-3-6-4(5)7/h2-3H2,1H3,(H3,5,6,7)
InchiKey:	ZQZJKHIIQFPZCS-UHFFFAOYSA-N
Formula:	C4H10N2O
SMILES:	CCCNC(=N)O
Mol. weight [g/mol]:	102.14
CAS:	627-06-5

Physical Properties

Property code	Value	Unit	Source
gf	138.97	kJ/mol	Joback Method
hf	-26.32	kJ/mol	Joback Method
hvap	59.69	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	0.479		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
tb	517.61	K	Joback Method
tf	317.10	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	38.33	J/mol×K	100.12	Joback Method
cpg	201.84	J/mol×K	517.61	Joback Method

psub	1.76e-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	1.58e-03	kPa	354.10	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	1.08e-03	kPa	350.20	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	2.17e-03	kPa	357.30	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	9.90e-04	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	9.40e-04	kPa	348.70	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	7.40e-04	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	7.20e-04	kPa	345.70	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	4.70e-04	kPa	342.20	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	3.00e-04	kPa	337.40	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	1.90e-04	kPa	333.20	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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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 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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point