N-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

Physical Properties

Property code	Value	Unit	Source
gf	9.72	kJ/mol	Joback Method
hf	-151.21	kJ/mol	Joback Method
hfus	18.01	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.065		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	467.49	K	Joback Method
tc	665.92	K	Joback Method
tf	320.69	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.41	J/mol×K	467.49	Joback Method
cpg	198.33	J/mol×K	500.56	Joback Method
cpg	206.83	J/mol×K	533.63	Joback Method
cpg	214.91	J/mol×K	566.71	Joback Method
cpg	222.59	J/mol×K	599.78	Joback Method
cpg	229.88	J/mol×K	632.85	Joback Method
cpg	236.79	J/mol×K	665.92	Joback Method

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
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	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	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	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	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	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	1.76e-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	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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

Legend

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