

Urea, N,N-diethyl-

Other names:	1,1-diethylurea Asym-Diethylurea N,N-diethylurea urea, 1,1-diethyl-
Inchi:	InChI=1S/C5H12N2O/c1-3-7(4-2)5(6)8/h3-4H2,1-2H3,(H2,6,8)
InchiKey:	TUMNHQRORINJKE-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CCN(CC)C(N)=O
Mol. weight [g/mol]:	116.16
CAS:	634-95-7

Physical Properties

Property code	Value	Unit	Source
chs	-3310.32 ± 0.89	kJ/mol	NIST Webbook
gf	39.53	kJ/mol	Joback Method
hf	-272.30 ± 1.60	kJ/mol	NIST Webbook
hfs	-372.20 ± 1.10	kJ/mol	NIST Webbook
hfus	18.52	kJ/mol	Joback Method
hsub	95.70 ± 0.70	kJ/mol	NIST Webbook
hvap	46.15	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.407		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	452.64	K	Joback Method
tc	643.84	K	Joback Method
tf	342.30 ± 0.40	K	NIST Webbook
tf	348.43 ± 0.02	K	NIST Webbook
tt	348.00 ± 0.00	K	NIST Webbook
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	218.82	J/molxK	452.64	Joback Method
cpg	266.82	J/molxK	611.97	Joback Method
cpg	258.20	J/molxK	580.10	Joback Method
cpg	249.11	J/molxK	548.24	Joback Method
cpg	239.52	J/molxK	516.37	Joback Method
cpg	229.43	J/molxK	484.51	Joback Method
cpg	274.99	J/molxK	643.84	Joback Method
cps	185.20	J/molxK	300.00	NIST Webbook
hfust	16.78	kJ/mol	342.30	NIST Webbook
hfust	16.78	kJ/mol	342.30	NIST Webbook
hsubt	95.50 ± 0.80	kJ/mol	326.00	NIST Webbook
hsubt	96.80	kJ/mol	326.00	NIST Webbook
hsubt	94.90 ± 0.80	kJ/mol	326.00	NIST Webbook
hsubt	94.70 ± 0.20	kJ/mol	350.00	NIST Webbook
hsubt	99.90 ± 1.10	kJ/mol	320.00	NIST Webbook
psub	6.20e-04	kPa	312.20	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	339.10	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	8.94e-03	kPa	336.70	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	6.10e-03	kPa	333.00	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	4.53e-03	kPa	330.20	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	3.89e-03	kPa	329.20	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	3.53e-03	kPa	328.20	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	2.90e-03	kPa	326.20	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	2.28e-03	kPa	324.20	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	1.50e-03	kPa	320.20	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	1.50e-03	kPa	320.10	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	1.06e-03	kPa	316.70	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	8.80e-04	kPa	315.20	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	6.80e-04	kPa	313.10	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	49.00	J/mol×K	342.30	NIST Webbook
ssubt	296.90	J/mol×K	326.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C634957&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 measurements	https://www.doi.org/10.1016/j.jct.2014.07.012
Measurement and Prediction of Thermochemical Properties: Improved Joback Method	https://www.doi.org/10.1021/je050230z
Increments for the Estimation of Enthalpies of Sublimation and Standard Enthalpies of Formation of Alkyl Derivatives of Urea:	https://en.wikipedia.org/wiki/Joback_method
	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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