

N,N'-Trimethyleneurea

Other names:	2(1H)-Pyrimidinone, tetrahydro- 2(1H)-Tetrahydropyrimidinone 2-Ketohexahydropyrimidine 2-Pyrimidinol, 3,4,5,6-tetrahydro- Hexahydro-2(1H)-pyrimidinone Hexahydropyrimidin-2-one NSC 21315 Propyleneurea Pyrimidine, hexahydro-2-oxo- Tetrahydro-2-pyrimidone Urea, 1,3-trimethylene- Urea, N,N'-(1,3-propanediyl)- perhydropyrimidin-2-one tetrahydropyrimidin-2(1H)-one
Inchi:	InChI=1S/C4H8N2O/c7-4-5-2-1-3-6-4/h1-3H2,(H2,5,6,7)
InchiKey:	NQPJDJVGBDHCAD-UHFFFAOYSA-N
Formula:	C4H8N2O
SMILES:	OC1=NCCCN1
Mol. weight [g/mol]:	100.12
CAS:	1852-17-1

Physical Properties

Property code	Value	Unit	Source
gf	102.96	kJ/mol	Joback Method
hf	-48.37	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	55.84	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	-0.106		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	6663.89	kPa	Joback Method
tb	513.71	K	Joback Method
tc	734.47	K	Joback Method
tf	397.13	K	Joback Method
vc	0.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.45	J/molxK	513.71	Joback Method
cpg	189.15	J/molxK	550.50	Joback Method
cpg	199.31	J/molxK	587.30	Joback Method
cpg	208.94	J/molxK	624.09	Joback Method
cpg	218.02	J/molxK	660.88	Joback Method
cpg	226.54	J/molxK	697.67	Joback Method
cpg	234.50	J/molxK	734.47	Joback Method
cps	155.10	J/molxK	350.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	118.00	J/molxK	270.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	120.10	J/molxK	275.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	122.20	J/molxK	280.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	124.10	J/molxK	285.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	126.20	J/molxK	290.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

cps	128.10	J/molxK	295.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	129.50	J/molxK	298.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	130.40	J/molxK	300.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	132.70	J/molxK	305.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	135.30	J/molxK	310.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	137.80	J/molxK	315.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	140.20	J/molxK	320.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	142.60	J/molxK	325.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	145.10	J/molxK	330.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

cps	147.30	J/mol×K	335.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	150.10	J/mol×K	340.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	152.20	J/mol×K	345.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	117.20	J/mol×K	268.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	157.20	J/mol×K	355.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	159.90	J/mol×K	360.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	163.80	J/mol×K	365.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	166.50	J/mol×K	370.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

cps	169.80	J/mol×K	375.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	172.40	J/mol×K	380.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	175.10	J/mol×K	385.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	177.30	J/mol×K	390.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	180.40	J/mol×K	395.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	183.30	J/mol×K	400.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	186.50	J/mol×K	405.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	189.80	J/mol×K	410.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	193.90	J/mol×K	415.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

cps	197.10	J/mol×K	420.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	200.80	J/mol×K	425.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	202.70	J/mol×K	430.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	204.90	J/mol×K	435.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	207.50	J/mol×K	440.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	210.30	J/mol×K	445.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	213.30	J/mol×K	450.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	215.90	J/mol×K	455.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

cps	219.10	J/mol×K	460.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	222.20	J/mol×K	465.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea
cps	224.90	J/mol×K	470.15	Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1852171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Structural studies of cyclic ureas: 1. Enthalpies of formation of imidazolidin-2-one and N,N0-trimethyleneurea:	https://www.doi.org/10.1016/j.jct.2007.08.004
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
cps:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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