Methenamine

Other names:

1,3,5,7-Tetraazaadamantane
1,3,5,7-Tetraazatricyclo-[3.3.1.1(3,7)]decane
1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane
1,3,5,7-tetraazatricyclo[3.3.1.1(3,7)]decane
AMMOFORM
AMMONIOFORMALDEHYDE
Aceto HMT
Aminoform
Aminoformaldehyde
Antihydral
Cystamin
Cystogen
DUIREXOL
Ekagom H
Formamine
Formin
Formin (heterocycle)
H.M.T.
HEXAMETHYLENETETRAMINE
HMT
Herax UTS
Heterin
Hexa
Hexa-Flo-Pulver
Hexaform
Hexaloids
Hexamethylenamine
Hexamethylenetetraamine
Hexamethylentetramin
Hexamine
Hexamine (heterocycle)
Hexasan
Hexilmethylenamine
Methenamin
Metramine
Nocceler H
Preparation AF
Resotropin
Sanceler H
Uramin

	Uratrine
	Uritone
	Urodeine
	Urotropin
	Urotropine
	Vesaloin
	Vulkacit H 30
	Xametrin
Inchi:	InChI=1S/C6H12N4/c1-7-2-9-4-8(1)5-10(3-7)6-9/h1-6H2
InchiKey:	VKYKSIONXSXAKP-UHFFFAOYSA-N
Formula:	C6H12N4
SMILES:	C1N2CN3CN1CN(C2)C3
Mol. weight [g/mol]:	140.19
CAS:	100-97-0

Physical Properties

Property code	Value	Unit	Source
chs	-4199.10	kJ/mol	NIST Webbook
chs	-4200.11 ± 0.67	kJ/mol	NIST Webbook
hf	197.90	kJ/mol	NIST Webbook
hf	199.00 ± 3.00	kJ/mol	NIST Webbook
hfs	123.00	kJ/mol	NIST Webbook
hfs	124.10 ± 0.75	kJ/mol	NIST Webbook
hsub	79.60 ± 0.40	kJ/mol	NIST Webbook
hsub	74.90 ± 2.90	kJ/mol	NIST Webbook
hsub	74.90	kJ/mol	NIST Webbook
hsub	75.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.55	eV	NIST Webbook
ie	8.26	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
log10ws	0.73		Crippen Method
logp	-1.020		Crippen Method
mcvol	102.740	ml/mol	McGowan Method
rinpol	1210.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	206.78		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	2014.00		NIST Webbook

ripol	2014.00		NIST Webbook
ss	163.38	J/mol×K	NIST Webbook
ss	163.38	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	152.29	J/mol×K	298.15	NIST Webbook
cps	152.29	J/mol×K	298.15	NIST Webbook
hsubt	77.70 ± 0.40	kJ/mol	358.50	NIST Webbook
hsubt	76.80	kJ/mol	375.50	NIST Webbook
hsubt	78.80	kJ/mol	315.00	NIST Webbook
hsubt	74.10 ± 0.80	kJ/mol	289.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.14393e+01
Coeff. B	-9.23798e+03
Coeff. C	-2.54812e-05
Coeff. D	3.10254e-11
Temperature range (K), min.	298.15
Temperature range (K), max.	453.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Hexamethylenetetramine in a Pure Water, Methanol, Acetic Acid, and Ethanol + Water Mixture from (299.38 to 340.35) K:	https://www.doi.org/10.1021/je800662m
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density, Speed of Sound, Viscosity, and Surface Tension of Hexamethylenetetramine Aqueous Solutions from T = (298.15 to 329.15) K:	https://www.doi.org/10.1021/acs.jced.8b00492
Heat Capacities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures:	https://www.doi.org/10.1021/je9006579
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1325

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1325
Thermochemistry of hexamethylenetetramine pentaborate:	https://www.doi.org/10.1016/j.tca.2005.08.021
Densities and Viscosities of Binary Mixtures of Acetic Acid with Acetic Anhydride and Methenamine at Different Temperatures:	https://www.doi.org/10.1021/je8003782
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100970&Units=SI
Solubility of 1,3,5,7-tetra azatricyclo[3.3.1.13,7]decane (HMT) in water from 275.15K to 313.15K:	https://www.doi.org/10.1016/j.tca.2006.08.010

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions