Hexamethylenimine

Other names:	1-Azacycloheptane 1H-Azepine, hexahydro- AZACYCLOHEPTANE Azepan Azepine, hexahydro- CYCLOHEXAMETHYLENIMINE G 0 HEXAHYDROAZEPINE Hexahydro-1H-azepine Hexamethyleneimine Homopiperidine NSC 16236 Perhydroazepine UN 2493
Inchi:	InChI=1S/C6H13N/c1-2-4-6-7-5-3-1/h7H,1-6H2
InchiKey:	ZSIQJIWKELUFRJ-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	C1CCCNCC1
Mol. weight [g/mol]:	99.17
CAS:	111-49-9

Physical Properties

Property code	Value	Unit	Source
affp	956.70	kJ/mol	NIST Webbook
basg	923.50	kJ/mol	NIST Webbook
chl	-4129.70 ± 1.60	kJ/mol	NIST Webbook
gf	107.41	kJ/mol	Joback Method
hf	-45.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-89.30 ± 1.60	kJ/mol	NIST Webbook
hfus	9.55	kJ/mol	Joback Method
hvap	44.30	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.41 ± 0.02	eV	NIST Webbook
log10ws	-1.42		Crippen Method
logp	1.150		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method

rinpol	864.00		NIST Webbook
rinpol	864.00		NIST Webbook
ripol	1178.00		NIST Webbook
tb	413.72	K	Joback Method
tc	637.36	K	Joback Method
tf	270.51	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.71	J/mol×K	637.36	Joback Method
cpg	218.67	J/mol×K	525.54	Joback Method
cpg	232.43	J/mol×K	562.81	Joback Method
cpg	245.44	J/mol×K	600.09	Joback Method
cpg	172.71	J/mol×K	413.72	Joback Method
cpg	188.82	J/mol×K	450.99	Joback Method
cpg	204.13	J/mol×K	488.27	Joback Method
cpl	205.00	J/mol×K	298.00	NIST Webbook
hvapt	40.40	kJ/mol	361.50	NIST Webbook
hvapt	37.70	kJ/mol	385.50	NIST Webbook
pvap	1.90	kPa	307.85	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	2.54	kPa	313.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	2.52	kPa	313.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.43	kPa	283.74	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.26	kPa	275.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.32	kPa	278.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.40	kPa	281.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.49	kPa	284.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.60	kPa	287.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.74	kPa	290.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.90	kPa	293.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.05	kPa	296.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.52	kPa	302.20	Vapour pressure and enthalpy of vaporization of cyclic imines

pvap	1.82	kPa	305.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	2.18	kPa	308.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	2.41	kPa	311.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	3.02	kPa	314.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	3.48	kPa	317.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	4.04	kPa	321.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.20	kPa	273.13	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.33	kPa	279.54	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.43	kPa	283.73	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	2.53	kPa	313.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.62	kPa	289.07	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.81	kPa	293.28	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.09	kPa	298.24	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.41	kPa	302.35	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

rhol	887.77	kg/m3	285.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	839.72	kg/m3	339.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	839.27	kg/m3	340.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	838.82	kg/m3	340.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	898.81	kg/m3	273.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	898.36	kg/m3	273.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	897.92	kg/m3	274.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	897.48	kg/m3	274.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	897.04	kg/m3	275.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	896.60	kg/m3	275.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	896.16	kg/m3	276.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	895.72	kg/m3	276.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	895.28	kg/m3	277.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	894.84	kg/m3	277.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	894.40	kg/m3	278.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	893.96	kg/m3	278.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	893.51	kg/m3	279.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	893.07	kg/m3	279.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	892.63	kg/m3	280.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	892.19	kg/m3	280.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	891.75	kg/m3	281.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	891.31	kg/m3	281.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	890.87	kg/m3	282.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	890.42	kg/m3	282.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	889.98	kg/m3	283.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	889.54	kg/m3	283.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	889.10	kg/m3	284.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	888.66	kg/m3	284.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	888.22	kg/m3	285.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	838.37	kg/m3	341.16	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	887.33	kg/m3	286.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	886.89	kg/m3	286.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	886.45	kg/m3	287.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	886.00	kg/m3	287.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	885.56	kg/m3	288.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	885.12	kg/m3	288.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	884.68	kg/m3	289.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	884.23	kg/m3	289.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	883.79	kg/m3	290.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	883.35	kg/m3	290.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	882.91	kg/m3	291.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	882.47	kg/m3	291.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	882.03	kg/m3	292.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	881.58	kg/m3	292.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	881.15	kg/m3	293.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	880.71	kg/m3	293.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	880.26	kg/m3	294.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	879.82	kg/m3	294.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	879.38	kg/m3	295.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	878.94	kg/m3	295.65	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	858.06	kg/m3	319.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	857.61	kg/m3	319.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	857.17	kg/m3	320.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	856.72	kg/m3	320.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	856.28	kg/m3	321.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	855.83	kg/m3	321.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	855.39	kg/m3	322.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	854.94	kg/m3	322.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	854.49	kg/m3	323.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	854.05	kg/m3	323.65	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	853.60	kg/m3	324.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	853.15	kg/m3	324.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	852.71	kg/m3	325.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	852.26	kg/m3	325.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	851.81	kg/m3	326.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	851.37	kg/m3	326.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	850.92	kg/m3	327.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	850.47	kg/m3	327.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	850.03	kg/m3	328.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	849.58	kg/m3	328.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	849.13	kg/m3	329.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	848.69	kg/m3	329.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	848.24	kg/m3	330.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	847.79	kg/m3	330.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	847.35	kg/m3	331.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	846.90	kg/m3	331.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	846.45	kg/m3	332.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	846.00	kg/m3	332.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	845.55	kg/m3	333.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	845.11	kg/m3	333.65	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	844.66	kg/m3	334.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	844.21	kg/m3	334.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	843.76	kg/m3	335.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	843.31	kg/m3	335.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	842.86	kg/m3	336.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	842.42	kg/m3	336.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	841.96	kg/m3	337.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	841.52	kg/m3	337.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	841.07	kg/m3	338.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	840.62	kg/m3	338.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhol	840.17	kg/m3	339.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhol	837.92	kg/m3	341.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
tcondl	0.13	W/m×K	333.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.13	W/m×K	313.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.14	W/m×K	293.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.14	W/m×K	273.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	99.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41849e+01
Coeff. B	-3.28808e+03
Coeff. C	-6.74930e+01
Temperature range (K), min.	304.09
Temperature range (K), max.	438.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05850e+02
Coeff. B	-9.05725e+03
Coeff. C	-1.33668e+01
Coeff. D	8.17005e-06
Temperature range (K), min.	236.15
Temperature range (K), max.	615.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1336
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1336.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111499&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open-Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576
Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine:	https://www.doi.org/10.1016/j.tca.2018.07.016
Joback Method:	https://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1021/je0498661
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://en.wikipedia.org/wiki/Joback_method
Volumetric properties of hexamethyleneimine and of its mixtures with water:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
	https://www.doi.org/10.1016/j.fluid.2014.12.017
	https://www.doi.org/10.1016/j.tca.2008.12.007

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization 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
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
vc:	Critical Volume