

# Hexamethylenimine

<b>Other names:</b>	1-Azacycloheptane 1H-Azepine, hexahydro- AZACYCLOHEPTANE Azepan Azepine, hexahydro- CYCLOHEXAMETHYLENIMINE G 0 HEXAHYDROAZEPINE Hexahydro-1H-azepine Hexamethyleneimine Homopiperidine NSC 16236 Perhydroazepine UN 2493
<b>Inchi:</b>	InChI=1S/C6H13N/c1-2-4-6-7-5-3-1/h7H,1-6H2
<b>InchiKey:</b>	ZSIQJIWKELUFRJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H13N
<b>SMILES:</b>	C1CCCNCC1
<b>Mol. weight [g/mol]:</b>	99.17
<b>CAS:</b>	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	8.41 ± 0.02	eV	NIST Webbook
ie	8.50	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	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.82	J/mol×K	450.99	Joback Method
cpg	218.67	J/mol×K	525.54	Joback Method
cpg	204.13	J/mol×K	488.27	Joback Method
cpg	172.71	J/mol×K	413.72	Joback Method
cpg	257.71	J/mol×K	637.36	Joback Method
cpg	245.44	J/mol×K	600.09	Joback Method
cpg	232.43	J/mol×K	562.81	Joback Method
cpl	205.00	J/mol×K	298.00	NIST Webbook
hvapt	37.70	kJ/mol	385.50	NIST Webbook
hvapt	40.40	kJ/mol	361.50	NIST Webbook
pvap	3.02	kPa	314.20	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	1.05	kPa	296.20	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	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	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	0.62	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
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	2.53	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	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	0.74	kPa	290.20	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	0.49	kPa	284.20	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	0.32	kPa	278.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.26	kPa	275.30	Vapour pressure and enthalpy of vaporization of cyclic imines

pvap	3.48	kPa	317.20	Vapour pressure and enthalpy of vaporization of cyclic imines
rhoI	884.23	kg/m3	289.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	895.28	kg/m3	277.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	894.84	kg/m3	277.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	894.40	kg/m3	278.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	893.96	kg/m3	278.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	893.51	kg/m3	279.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	893.07	kg/m3	279.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	892.63	kg/m3	280.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	892.19	kg/m3	280.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhoI	891.75	kg/m3	281.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	891.31	kg/m3	281.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	890.87	kg/m3	282.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	890.42	kg/m3	282.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	889.98	kg/m3	283.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	889.54	kg/m3	283.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	889.10	kg/m3	284.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	888.66	kg/m3	284.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	888.22	kg/m3	285.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	887.77	kg/m3	285.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhoI	887.33	kg/m3	286.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	886.89	kg/m3	286.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	886.45	kg/m3	287.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	886.00	kg/m3	287.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	885.56	kg/m3	288.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	885.12	kg/m3	288.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	884.68	kg/m3	289.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	895.72	kg/m3	276.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	883.79	kg/m3	290.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	883.35	kg/m3	290.66	Volumetric properties of hexamethyleneimine and of its mixtures with water



rho1	896.16	kg/m3	276.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	882.47	kg/m3	291.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	882.03	kg/m3	292.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	881.58	kg/m3	292.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	881.15	kg/m3	293.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	880.71	kg/m3	293.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	880.26	kg/m3	294.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	879.82	kg/m3	294.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	879.38	kg/m3	295.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rho1	878.94	kg/m3	295.65	Volumetric properties of hexamethyleneimine and of its mixtures with water

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

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

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

rhoI	844.66	kg/m3	334.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	844.21	kg/m3	334.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	843.76	kg/m3	335.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	843.31	kg/m3	335.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	842.86	kg/m3	336.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	896.60	kg/m3	275.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	841.96	kg/m3	337.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	841.52	kg/m3	337.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	841.07	kg/m3	338.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	840.62	kg/m3	338.66	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhoI	897.04	kg/m3	275.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	839.72	kg/m3	339.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	839.27	kg/m3	340.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	838.82	kg/m3	340.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	838.37	kg/m3	341.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	837.92	kg/m3	341.65	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	897.48	kg/m3	274.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	897.92	kg/m3	274.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	898.36	kg/m3	273.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	898.81	kg/m3	273.16	Volumetric properties of hexamethyleneimine and of its mixtures with water

rhoI	842.42	kg/m <sup>3</sup>	336.66	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	882.91	kg/m <sup>3</sup>	291.15	Volumetric properties of hexamethyleneimine and of its mixtures with water
rhoI	840.17	kg/m <sup>3</sup>	339.16	Volumetric properties of hexamethyleneimine and of its mixtures with water
tcondI	0.13	W/m×K	313.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondI	0.14	W/m×K	293.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondI	0.14	W/m×K	273.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondI	0.13	W/m×K	333.15	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	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols.

Crippen Method:

KDB:

Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, N-Ethylmaleimide, Tetrahydrothiophene, and Tetrahydrofuran and Enthalpy of vaporization of cyclic imines: Thermodynamic study of heptane + amine mixtures. V. Excess and volumetric properties of hexamethyleneimine and of its mixtures with water:

The Yaws Handbook of Vapor Pressure: 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/10.1021/acs.jced.6b00576>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1336>

[https://www.chemo.com/doc/models/crippen\\_log10ws](https://www.chemo.com/doc/models/crippen_log10ws)

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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C111499&Units=SI>

<https://www.doi.org/10.1016/j.tca.2018.07.016>

<https://www.doi.org/10.1016/j.fluid.2014.12.017>

<https://www.doi.org/10.1016/j.tca.2008.12.007>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1016/j.jct.2011.04.017>



## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rho:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tcondl:</b>	Liquid thermal conductivity
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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