1,6-Hexanediamine

Other names:	1,6-DIAMINO-N-HEXANE
	1,6-Diaminohexane
	1,6-Hexamethylenediamine
	1,6-Hexylenediamine
	H2N(CH2)6NH2
	HEXYLENEDIAMINE
	HMDA
	Hexamethylenediamine
	NCI-C61405
	NSC 9257
	UN 2280
Inchi:	InChI=1S/C6H16N2/c7-5-3-1-2-4-6-8/h1-8H2
InchiKey:	NAQMVNRVTILPCV-UHFFFAOYSA-N
Formula:	C6H16N2
SMILES:	NCCCCCCN
Mol. weight [g/mol]:	116.20
CAS:	124-09-4

Physical Properties

Property code	Value	Unit	Source
affp	1008.00	kJ/mol	NIST Webbook
affp	980.30	kJ/mol	NIST Webbook
affp	999.50	kJ/mol	NIST Webbook
basg	946.20	kJ/mol	NIST Webbook
gf	132.54	kJ/mol	Joback Method
hf	-99.59	kJ/mol	Joback Method
hfs	-205.00	kJ/mol	NIST Webbook
hfus	59.62	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.28	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.16	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	61.08	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.06	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.01	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.94	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.83	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.75	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.72	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.62	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.44	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.29	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.13	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	60.07	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.84	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.82	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.38	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	59.51	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.39	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.32	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.20	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.17	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	59.05	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.90	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.74	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.56	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.28	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.97	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	39.38	kJ/mol	Solid-Liquid Equilibria of Naphthalene + Alkanediamine Mixtures
hfus	61.38	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	50.23	kJ/mol	Joback Method
ie	7.52	eV	NIST Webbook
log10ws	-1.20		Crippen Method
logp	0.464		Crippen Method
mcvol	115.360	ml/mol	McGowan Method

pc	3590.00	kPa	Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12)
tb	477.70	K	NIST Webbook
tc	674.62	K	Joback Method
tf	323.90	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.30	J/mol×K	481.74	Joback Method
cpg	277.23	J/mol×K	513.89	Joback Method
cpg	288.61	J/mol×K	546.03	Joback Method
cpg	299.47	J/mol×K	578.18	Joback Method
cpg	309.82	J/mol×K	610.33	Joback Method
cpg	319.67	J/mol×K	642.48	Joback Method
cpg	329.05	J/mol×K	674.62	Joback Method
cpl	301.42	J/mol×K	317.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	301.25	J/mol×K	315.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	301.08	J/mol×K	314.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	301.59	J/mol×K	318.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	301.77	J/mol×K	320.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	301.95	J/mol×K	321.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	302.14	J/mol×K	323.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	302.33	J/mol×K	324.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	302.53	J/mol×K	326.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	302.74	J/mol×K	327.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	302.95	J/mol×K	329.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	303.17	J/mol×K	330.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	303.40	J/mol×K	332.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	303.64	J/mol×K	333.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	303.88	J/mol×K	335.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	304.13	J/mol×K	336.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	304.40	J/mol×K	338.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	304.67	J/mol×K	339.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	304.95	J/mol×K	341.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	305.25	J/mol×K	342.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	305.55	J/mol×K	344.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	305.87	J/mol×K	345.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	306.20	J/mol×K	347.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	306.54	J/mol×K	348.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	306.89	J/mol×K	350.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	307.26	J/mol×K	351.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	307.64	J/mol×K	353.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
hfust	39.38	kJ/mol	311.60	NIST Webbook
hfust	40.21	kJ/mol	312.30	NIST Webbook
hvapt	49.30	kJ/mol	411.00	NIST Webbook
hvapt	51.30	kJ/mol	405.50	NIST Webbook
psub	5.20e-04	kPa	278.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.50e-04	kPa	278.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.40e-04	kPa	278.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.22e-03	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.22e-03	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	1.22e-03	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.61e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.61e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.61e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.70e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.70e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.76e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.46e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.47e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	5.48e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.85e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.85e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.87e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.08	kPa	313.51	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	0.02	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	303.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	303.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	303.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.03	kPa	306.00	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.03	kPa	306.00	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.04	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.04	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	0.04	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.08	kPa	313.51	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
rhol	856.20	kg/m3	313.15	Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine
rhol	850.00	kg/m3	318.15	Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine
rhol	845.30	kg/m3	323.15	Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine

rhol	842.30	kg/m3	328.15	Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine
rhol	838.10	kg/m3	333.15	Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52423e+01
Coeff. B	-4.30331e+03
Coeff. C	-7.26440e+01
Temperature range (K), min.	360.40
Temperature range (K), max.	505.97

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.58003e+02
Coeff. B	-1.79905e+04
Coeff. C	-3.57701e+01
Coeff. D	2.20695e-05
Temperature range (K), min.	313.95
Temperature range (K), max.	663.00

Sources

Vapor-liquid equilibrium measurement and ENRTL Modeling of CO2 absorption in aqueous hexamethylenediamine:	https://www.doi.org/10.1016/j.fluid.2015.05.033
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1329.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124094&Units=SI
Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12):	https://www.doi.org/10.1021/je050424e
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities and Viscosities of (1,6-Hexanediamine + Ethanol) and (1,6-Hexanediamine + Ethanol + Water) at T = (303.15 to 328.15) K:	https://www.doi.org/10.1021/je800942u
Liquid-Liquid Equilibria Determination and Prediction for Ternary Systems of Water + 1,6-Hexanediamine + (1-Butanol or 1-Pentanol) at 298.2, 308.2, and 318.2 K:	https://www.doi.org/10.1021/acs.jced.7b00678
NDRL/Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1329
Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties:	https://www.doi.org/10.1016/j.fluid.2014.03.013
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental measurement and Kent-Eisenberg modelling of CO2 solubility in aqueous mixture of 2-amino-2-methyl-1-propanol and hexamethylenediamine:	https://www.doi.org/10.1016/j.jct.2011.06.008
Joback Method:	https://www.doi.org/10.1016/j.fluid.2017.01.020
The Yaws Handbook of Vapor Pressure:	https://en.wikipedia.org/wiki/Joback_method
Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Solid-Liquid Equilibria of Naphthalene + Alkanediamine Mixtures:	https://www.doi.org/10.1021/je900537y
	https://www.doi.org/10.1021/je0502851

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid 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
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
psub:	Sublimation pressure

pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume