H2N(CH2)7NH2

Other names: 1,7-Diaminoheptane
1,7-Heptamethylenediamine
1,7-Heptanediamine
Heptamethylenediamine
Inchi: InChI=1S/C7H18N2/c8-6-4-2-1-3-5-7-9/h1-9H2
InchiKey: PWSKHLMYTZNYKO-UHFFFAOYSA-N
Formula: C7H18N2
SMILES: NCCCCCCCN
Mol. weight [g/mol]: 130.23
CAS: 646-19-5

Physical Properties

Property code	Value	Unit	Source
affp	998.50	kJ/mol	NIST Webbook
basg	944.90	kJ/mol	NIST Webbook
basg	922.00 ± 3.00	kJ/mol	NIST Webbook
gf	140.96	kJ/mol	Joback Method
hf	-120.23	kJ/mol	Joback Method
hfus	63.04	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.35	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.27	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.75	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	62.03	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	62.24	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	62.36	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	62.71	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	62.73	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.33	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.10	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.09	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.63	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.42	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.15	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.74	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.66	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.66	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.18	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.06	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	63.69	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	63.38	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	63.21	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	61.69	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	52.46	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.854		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
ripol	1744.00		NIST Webbook
tb	497.20	K	NIST Webbook
tc	695.22	K	Joback Method
tf	335.17	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.55	J/mol×K	504.62	Joback Method
cpg	321.48	J/mol×K	536.39	Joback Method
cpg	333.83	J/mol×K	568.15	Joback Method
cpg	345.60	J/mol×K	599.92	Joback Method
cpg	356.81	J/mol×K	631.69	Joback Method
cpg	367.49	J/mol×K	663.45	Joback Method
cpg	377.66	J/mol×K	695.22	Joback Method
cpl	341.76	J/mol×K	353.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	332.76	J/mol×K	302.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	333.11	J/mol×K	305.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	333.29	J/mol×K	306.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	333.48	J/mol×K	308.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	333.67	J/mol×K	309.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	333.86	J/mol×K	311.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	334.06	J/mol×K	312.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	334.27	J/mol×K	314.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	334.48	J/mol×K	315.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	334.70	J/mol×K	317.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	334.92	J/mol×K	318.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	335.15	J/mol×K	320.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	335.38	J/mol×K	321.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	335.62	J/mol×K	323.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	335.87	J/mol×K	324.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	336.12	J/mol×K	326.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	336.38	J/mol×K	327.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	336.64	J/mol×K	329.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	336.91	J/mol×K	330.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	337.18	J/mol×K	332.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	337.47	J/mol×K	333.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	337.76	J/mol×K	335.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	338.05	J/mol×K	336.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	338.35	J/mol×K	338.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	338.66	J/mol×K	339.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	338.98	J/mol×K	341.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	339.30	J/mol×K	342.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	339.63	J/mol×K	344.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	339.97	J/mol×K	345.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	340.31	J/mol×K	347.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	340.66	J/mol×K	348.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	341.02	J/mol×K	350.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	341.39	J/mol×K	351.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	332.93	J/mol×K	303.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
hfust	36.95	kJ/mol	298.50	NIST Webbook
hvapt	46.50	kJ/mol	293.00	NIST Webbook
psub	1.78e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	2.20e-04	kPa	273.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.20e-04	kPa	273.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.30e-04	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.30e-04	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.30e-04	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	8.70e-04	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	8.70e-04	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	8.60e-04	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.79e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	1.79e-03	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.20e-04	kPa	273.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.61e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.62e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.61e-03	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.81e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.82e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.82e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	3.81e-03	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.49e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.48e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.48e-03	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.85e-03	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.86e-03	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.87e-03	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.56908e+01
Coeff. B	-4.62653e+03
Coeff. C	-7.93580e+01
Temperature range (K), min.	379.72
Temperature range (K), max.	525.10

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines:	https://www.doi.org/10.1016/j.jct.2011.06.008
Joback Method:	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.doi.org/10.1021/je900537y
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1420.mol
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

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
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
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
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume