1,3-Propanediamine

Other names:	1,3-Diaminopropane
	1,3-Propylenediamine
	H2N(CH2)3NH2
	Propane-1,3-diamine
	Trimethylenediamine
Inchi:	InChI=1S/C3H10N2/c4-2-1-3-5/h1-5H2
InchiKey:	XFNJVJPLKCPIBV-UHFFFAOYSA-N
Formula:	C3H10N2
SMILES:	NCCCN
Mol. weight [g/mol]:	74.12
CAS:	109-76-2

Physical Properties

Property code	Value	Unit	Source
affp	970.70	kJ/mol	NIST Webbook
affp	982.40	kJ/mol	NIST Webbook
affp	987.00	kJ/mol	NIST Webbook
affp	978.00 ± 4.00	kJ/mol	NIST Webbook
basg	940.00	kJ/mol	NIST Webbook
gf	107.28	kJ/mol	Joback Method
hf	-37.67	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	49.10	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	48.79	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	49.42	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	49.74	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	47.84	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	47.52	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	50.03	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	50.36	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	50.68	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	50.97	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	51.30	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	48.47	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	50.16 ± 0.10	kJ/mol	NIST Webbook
hvap	50.20 ± 0.10	kJ/mol	NIST Webbook
hvap	50.18	kJ/mol	NIST Webbook
log10ws	0.05		Crippen Method
logp	-0.706		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
pc	5590.00	kPa	Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12)
rinpol	720.00		NIST Webbook
rinpol	748.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1337.00		NIST Webbook
tb	413.20	K	NIST Webbook
tb	412.85	K	NIST Webbook
tb	412.90	K	NIST Webbook
tc	612.43	K	Joback Method
tf	249.65 ± 0.50	K	NIST Webbook

tf	261.20 ± 0.60	K	NIST Webbook
tf	261.15	K	NIST Webbook
vc	0.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.67	J/mol×K	612.43	Joback Method
cpg	156.37	J/mol×K	446.32	Joback Method
cpg	164.11	J/mol×K	479.54	Joback Method
cpg	171.50	J/mol×K	512.76	Joback Method
cpg	178.55	J/mol×K	545.99	Joback Method
cpg	185.27	J/mol×K	579.21	Joback Method
cpg	148.26	J/mol×K	413.10	Joback Method
cpl	207.80	J/mol×K	338.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	208.30	J/mol×K	343.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	208.90	J/mol×K	348.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	209.50	J/mol×K	353.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends

cpl	203.05	J/mol×K	293.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.21	J/mol×K	294.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.37	J/mol×K	296.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.53	J/mol×K	297.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.59	J/mol×K	298.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.70	J/mol×K	299.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.86	J/mol×K	300.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	204.03	J/mol×K	302.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	204.19	J/mol×K	303.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	204.36	J/mol×K	305.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	204.53	J/mol×K	306.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	204.70	J/mol×K	308.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	204.87	J/mol×K	309.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	205.04	J/mol×K	311.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	205.21	J/mol×K	312.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	205.38	J/mol×K	314.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	205.56	J/mol×K	315.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	205.73	J/mol×K	317.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	205.91	J/mol×K	318.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	206.08	J/mol×K	320.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	206.26	J/mol×K	321.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	206.43	J/mol×K	323.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	206.61	J/mol×K	324.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	206.79	J/mol×K	326.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	206.96	J/mol×K	327.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	207.14	J/mol×K	329.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	207.32	J/mol×K	330.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	207.50	J/mol×K	332.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	207.67	J/mol×K	333.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	207.85	J/mol×K	335.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	208.03	J/mol×K	336.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	208.20	J/mol×K	338.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	208.38	J/mol×K	339.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	208.56	J/mol×K	341.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	208.73	J/mol×K	342.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	208.91	J/mol×K	344.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	209.08	J/mol×K	345.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	209.26	J/mol×K	347.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	209.43	J/mol×K	348.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	209.60	J/mol×K	350.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	207.10	J/mol×K	333.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	209.95	J/mol×K	353.15	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K

cpl	206.50	J/mol×K	328.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	205.90	J/mol×K	323.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	205.30	J/mol×K	318.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	204.80	J/mol×K	313.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	204.20	J/mol×K	308.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
cpl	209.78	J/mol×K	351.65	Heat Capacities of Some Liquid a,?-Alkanediamines in the Temperature Range between (293.15 and 353.15) K
cpl	203.70	J/mol×K	303.20	Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends
hfust	12.19	kJ/mol	262.40	NIST Webbook

hvapt	40.85	kJ/mol	412.90	NIST Webbook
psub	2.11e-03	kPa	243.15	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	255.66	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	255.66	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	255.66	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	9.50e-04	kPa	238.12	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.10e-04	kPa	233.15	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.10e-04	kPa	233.15	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	9.50e-04	kPa	238.12	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	9.50e-04	kPa	238.12	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.11e-03	kPa	243.15	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.11e-03	kPa	243.15	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
pvap	12.67	kPa	354.83	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	19.47	kPa	364.78	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	8.26	kPa	344.87	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures

pvap	3.15	kPa	324.90	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	1.83	kPa	314.79	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	0.58	kPa	294.82	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	0.32	kPa	284.84	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	0.32	kPa	284.84	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures

pvap	5.17	kPa	334.87	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
rhol	879.81	kg/m3	298.15	Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56499e+01
Coeff. B	-3.94103e+03
Coeff. C	-5.59500e+01
Temperature range (K), min.	312.49
Temperature range (K), max.	437.15

Sources

Molar heat capacity of aqueous solutions of 1,3-diaminopropane and 1,4-diaminobutane and their piperazine blends:	https://www.doi.org/10.1016/j.tca.2015.08.003
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12):	https://www.doi.org/10.1021/je050424e
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
Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures:	https://www.doi.org/10.1016/j.jct.2010.12.010
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
Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K:	https://www.doi.org/10.1016/j.tca.2006.08.006
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1413.mol
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

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
rhol:	Liquid Density
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