1,2-Propanediamine

Other names: 1,2-DIAMINOPROPANE
1,2-Propylenediamine
PROPYLENEDIAMINE
UN 2258
Inchi: InChI=1S/C3H10N2/c1-3(5)2-4/h3H,2,4-5H2,1H3
InchiKey: AOHJOMMDDJHIJH-UHFFFAOYSA-N
Formula: C3H10N2
SMILES: CC(N)CN
Mol. weight [g/mol]: 74.12
CAS: 78-90-0

Physical Properties

Property code	Value	Unit	Source
chl	-2511.90 ± 0.30	kJ/mol	NIST Webbook
gf	104.84	kJ/mol	Joback Method
hf	-53.60 ± 0.46	kJ/mol	NIST Webbook
hfl	-97.80 ± 0.40	kJ/mol	NIST Webbook
hfus	10.40	kJ/mol	Joback Method
hvap	43.90 ± 0.20	kJ/mol	NIST Webbook
hvap	44.20 ± 0.20	kJ/mol	NIST Webbook
hvap	44.20	kJ/mol	NIST Webbook
hvap	44.20 ± 0.20	kJ/mol	NIST Webbook
hvap	43.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.06		Crippen Method
logp	-0.708		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
ripol	1199.00		NIST Webbook
ripol	1201.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1201.00		NIST Webbook
ripol	1225.00		NIST Webbook
sl	247.27	J/mol×K	NIST Webbook
tb	392.70	K	NIST Webbook
tb	394.10	K	NIST Webbook
tb	390.50 ± 0.30	K	NIST Webbook

tc	616.86	K	Joback Method
tf	236.00 ± 0.60	K	NIST Webbook
tf	236.00	K	NIST Webbook
tt	236.53 ± 0.03	K	NIST Webbook
tt	236.53 ± 0.03	K	NIST Webbook
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.14	J/mol×K	616.86	Joback Method
cpg	156.74	J/mol×K	446.69	Joback Method
cpg	164.75	J/mol×K	480.73	Joback Method
cpg	172.39	J/mol×K	514.76	Joback Method
cpg	179.66	J/mol×K	548.79	Joback Method
cpg	186.57	J/mol×K	582.83	Joback Method
cpg	148.34	J/mol×K	412.66	Joback Method
cpl	205.64	J/mol×K	298.15	NIST Webbook
hfust	18.42	kJ/mol	236.50	NIST Webbook
hfust	0.07	kJ/mol	222.00	NIST Webbook
hfust	18.42	kJ/mol	236.50	NIST Webbook
hvapt	47.20	kJ/mol	267.50	NIST Webbook
hvapt	47.20	kJ/mol	267.50	NIST Webbook
hvapt	42.20	kJ/mol	343.00	NIST Webbook
pvap	1.56	kPa	299.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	2.10	kPa	303.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	2.07	kPa	303.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.84	kPa	301.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	1.82	kPa	301.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.59	kPa	284.01	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	1.15	kPa	293.98	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	1.15	kPa	293.98	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	1.15	kPa	293.98	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures

pvap	2.10	kPa	303.91	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	2.10	kPa	303.91	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	2.10	kPa	303.91	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	3.67	kPa	313.84	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	3.67	kPa	313.84	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures

pvap	3.66	kPa	313.84	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	6.24	kPa	324.02	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	10.11	kPa	334.00	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	36.31	kPa	363.91	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
pvap	2.35	kPa	305.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.27	kPa	273.80	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	0.30	kPa	274.90	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.34	kPa	276.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.35	kPa	277.00	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.40	kPa	279.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.42	kPa	279.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.46	kPa	281.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.53	kPa	282.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.52	kPa	283.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.62	kPa	285.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.63	kPa	285.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	0.72	kPa	287.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.79	kPa	288.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.83	kPa	289.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.95	kPa	291.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.95	kPa	291.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.07	kPa	293.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.19	kPa	294.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.23	kPa	295.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.36	kPa	297.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.42	kPa	297.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	1.63	kPa	299.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	36.33	kPa	363.91	Phase equilibrium properties of binary aqueous solutions containing ethanediamine, 1,2-diaminopropane, 1,3-diaminopropane, or 1,4-diaminobutane at several temperatures
rhol	857.09	kg/m3	298.15	Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K
sfust	77.89	J/mol×K	236.50	NIST Webbook
sfust	0.30	J/mol×K	222.00	NIST Webbook
srf	0.04	N/m	283.15	Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from T = (283.15 to 323.15) K
srf	0.03	N/m	323.15	Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from T = (283.15 to 323.15) K
srf	0.03	N/m	313.15	Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from T = (283.15 to 323.15) K

srf	0.03	N/m	303.15	Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from T = (283.15 to 323.15) K
srf	0.03	N/m	293.15	Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from T = (283.15 to 323.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53843e+01
Coeff. B	-3.62959e+03
Coeff. C	-5.55640e+01
Temperature range (K), min.	295.99
Temperature range (K), max.	415.90

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02248e+02
Coeff. B	-8.88258e+03
Coeff. C	-1.27764e+01
Coeff. D	8.48531e-06
Temperature range (K), min.	236.53
Temperature range (K), max.	587.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Surface Tension and Refractive Index of Benzylamine and 1,2-Diaminopropane Aqueous Solutions from (283.15 to 323.15) K:	https://www.doi.org/10.1021/je300382a
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
Benchmark thermodynamic properties of 1,x-alkanediamines: Experimental and theoretical study:	https://www.doi.org/10.1016/j.jct.2015.03.011
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/research/kdb/hcprop/showprop.php?cmpid=1261
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78900&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1261
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
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
pvap:	Vapor pressure
rhol:	Liquid Density
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume