1,3-Propanediamine, N,N-diethyl-

Other names:	(N,N-Diethylamino)propylamine
	1,3-Propanediamine, N1,N1-diethyl-
	1-(Diethylamino)propylamine-3
	1-Amino-3-(diethylamino)propane
	3-(Diethylamino)-1-propylamine
	3-(Diethylamino)propylamine
	3-(N,N-Diethylamino)-1-propylamine
	3-Diethylamino-n-propylamine
	3-aminopropyldiethylamine
	Diethylaminopropylamine
	Diethylaminotrimethylenamine
	N,N-Diethyl-1,3-diaminopropane
	N,N-Diethyl-1,3-propanediamine
	N,N-Diethylpropylenediamine
	N,N-Diethyltrimethylenediamine
	N,N-diethylpropane-1,3-diamine
	N-(3-Diethylaminopropyl)amine
	N-Diethyltrimethylenediamine
	NSC 7776
	UN 2684
	«gamma»-(Diethylamino)propylamine
	Â«gammaÂ»-(Diethylamino)propylamine
Inchi:	InChI=1S/C7H18N2/c1-3-9(4-2)7-5-6-8/h3-8H2,1-2H3
InchiKey:	QOHMWDJIBGVPIF-UHFFFAOYSA-N
Formula:	C7H18N2
SMILES:	CCN(CC)CCCN
Mol. weight [g/mol]:	130.23
CAS:	104-78-9

Physical Properties

Property code	Value	Unit	Source
gf	185.29	kJ/mol	Joback Method
hf	-86.49	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	43.86	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method

logp	0.677		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	442.55	K	NIST Webbook
tb	432.20	K	NIST Webbook
tb	441.70	K	NIST Webbook
tc	621.46	K	Joback Method
tf	284.38	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.24	J/mol×K	621.46	Joback Method
cpg	295.01	J/mol×K	474.02	Joback Method
cpg	343.47	J/mol×K	591.97	Joback Method
cpg	332.18	J/mol×K	562.48	Joback Method
cpg	320.35	J/mol×K	532.99	Joback Method
cpg	307.97	J/mol×K	503.51	Joback Method
cpg	281.45	J/mol×K	444.53	Joback Method
hvapt	52.40	kJ/mol	298.15	Vapor pressure and enthalpy of vaporization of aliphatic propanediamines
hvapt	46.40	kJ/mol	386.00	NIST Webbook
pvap	0.62	kPa	313.18	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.31	kPa	303.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}

pvap	0.59	kPa	313.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	1.05	kPa	323.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	1.81	kPa	333.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	2.99	kPa	343.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	4.76	kPa	353.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	7.35	kPa	363.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	0.01	kPa	263.16	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	0.03	kPa	273.05	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.08	kPa	283.27	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.08	kPa	283.27	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	0.16	kPa	293.22	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.33	kPa	303.14	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.33	kPa	303.16	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	0.62	kPa	313.16	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.15	kPa	293.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	1.11	kPa	323.16	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	1.11	kPa	323.16	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	1.94	kPa	333.18	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	3.23	kPa	343.21	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	5.16	kPa	353.19	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	5.16	kPa	353.19	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	7.96	kPa	363.25	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.03	kPa	273.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	0.08	kPa	283.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.16	kPa	293.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.33	kPa	303.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	0.62	kPa	313.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	1.11	kPa	323.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	1.92	kPa	333.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K

pvap	3.20	kPa	343.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	5.14	kPa	353.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	8.02	kPa	363.15	Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl 1,3-propanediamine at temperatures from 273 K to 363 K
pvap	0.07	kPa	283.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}
pvap	0.03	kPa	273.15	Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}

pvap	1.81	kPa	333.15	Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes)
pvap	1.05	kPa	323.15	Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes)
pvap	0.59	kPa	313.15	Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes)
pvap	0.31	kPa	303.15	Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes)
pvap	2.99	kPa	343.15	Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37437e+01
Coeff. B	-3.65186e+03
Coeff. C	-6.39290e+01
Temperature range (K), min.	302.05
Temperature range (K), max.	497.01

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapor pressure and enthalpy of vaporization of aliphatic propanediamines:	https://www.doi.org/10.1016/j.jct.2011.11.004
Excess properties and vapour pressure of (3-diethylaminopropylamine + n-alkanes):	https://www.doi.org/10.1016/j.jct.2008.01.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104789&Units=SI
Excess properties and vapour pressure of {3-diethylaminopropylamine + cyclohexane}:	https://www.doi.org/10.1016/j.jct.2010.01.016
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase equilibrium measurements and thermodynamic modeling of aqueous solutions of polyamines CO2 absorbents: 3-aminopropylmethylamine, 3-aminopropyldimethylamine and N,N-diethyl-1,3-propanediamine at temperatures from 273 K to 363 K:	https://www.doi.org/10.1016/j.jct.2015.08.023

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume