1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-

Other names:	1,3-Propanediamine, N1-(3-aminopropyl)-N1-methyl-
	1,7-diamino-4-methyl-4-azaheptane
	3,3'-diamino-N-methyldipropylamine
	3,3'-methyliminobispropylamine
	4-aza-4-methylheptane-1,7-diamine
	5-methyldipropylenetriamine
	Bis(«gamma»-aminopropyl)methylamine
	Bis(«omega»-aminopropyl)methylamine
	Di(«gamma»-aminopropyl)methylamine
	Methylamine, N,N-bis(3-aminopropyl)-
	N'-methyldipropylenetriamine
	N,N-Bis(«gamma»-aminopropyl)methylamine
	N,N-bis(.gamma.-aminopropyl)methylamine
	N,N-bis(3-aminopropyl)methylamine
	N-(3-aminopropyl)-N-methyl-1,3-propanediamine
	N-Methylbis(aminopropyl)amine
	N-Methyldipropylenetriamine
	N-Methyliminobis propylamine
	N-methyl-N,N-bis(3-aminopropyl)amine
	N-methyliminobis[1-propanamine]
	N-methyliminobis[propylamine]
	NSC 8173
	Propylamine, 3,3'-(methylimino)bis-
	bis(.gamma.-aminopropyl)methylamine
	bis(3-aminopropyl)methylamine
	di(.gamma.-aminopropyl)methylamine
	dipropylamine, 3,3'-diamino-N-methyl-
	methylbis(3-aminopropyl)amine
	methyliminobispropylamine
Inchi:	InChI=1S/C7H19N3/c1-10(6-2-4-8)7-3-5-9/h2-9H2,1H3
InchiKey:	KMBPCQSCMCEPMU-UHFFFAOYSA-N
Formula:	C7H19N3
SMILES:	CN(CCCN)CCCN
Mol. weight [g/mol]:	145.25
CAS:	105-83-9

Physical Properties

Property code	Value	Unit	Source
gf	251.74	kJ/mol	Joback Method
hf	-52.70	kJ/mol	Joback Method
hfus	27.30	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	-0.384		Crippen Method
mcvol	139.430	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	517.06	K	Joback Method
tc	705.41	K	Joback Method
tf	243.60 ± 0.60	K	NIST Webbook
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.14	J/mol×K	517.06	Joback Method
cpg	355.81	J/mol×K	548.45	Joback Method
cpg	368.82	J/mol×K	579.84	Joback Method
cpg	381.18	J/mol×K	611.23	Joback Method
cpg	392.92	J/mol×K	642.62	Joback Method
cpg	404.06	J/mol×K	674.02	Joback Method
cpg	414.63	J/mol×K	705.41	Joback Method
pvap	0.89	kPa	372.25	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	9.00e-03	kPa	303.24	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.02	kPa	313.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.02	kPa	313.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.04	kPa	323.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.04	kPa	323.36	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	0.09	kPa	333.37	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.09	kPa	333.37	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.17	kPa	343.43	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	0.32	kPa	353.36	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	0.56	kPa	363.42	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	4.00e-03	kPa	293.22	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	1.49	kPa	382.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	1.49	kPa	382.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	1.49	kPa	382.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	1.49	kPa	382.26	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	1.50	kPa	382.28	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	2.41	kPa	392.34	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	2.41	kPa	392.36	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	2.42	kPa	392.36	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	3.76	kPa	402.29	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	3.76	kPa	402.29	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	3.77	kPa	402.32	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	5.79	kPa	412.29	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	5.80	kPa	412.29	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	5.81	kPa	412.32	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	8.67	kPa	422.17	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	12.73	kPa	432.10	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

pvap	18.10	kPa	441.90	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N''-pentamethyldiethylenetriamine (PMDETA)) + water}
pvap	24.92	kPa	451.90	Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N''-pentamethyldiethylenetriamine (PMDETA)) + water}

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	0.80	NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapour-liquid equilibria, enthalpy of vaporisation, and excess Gibbs energies of binary mixtures of {3,3-diamino-N-methyldipropylamine (DNM) (or N,N,N',N''-pentamethyldiethylenetriamine (PMDETA)) + water}: https://www.doi.org/10.1016/j.jct.2018.08.025

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105839&Units=SI

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume