N,N,N',N'',N''-pentamethyldiethylenetriamine

Other names:	1,1,4,7,7-pentamethyl-1,4,7-triazaheptane
	1,1,4,7,7-pentamethyldiethylenetriamine
	N-[2-(dimethylamino)ethyl]-N,N',N'-trimethyl-1,2-ethanediamine
	N-methyl-N,N-bis(2-dimethylaminoethyl)amine
Inchi:	InChI=1S/C9H23N3/c1-10(2)6-8-12(5)9-7-11(3)4/h6-9H2,1-5H3
InchiKey:	UKODFQOELJFMII-UHFFFAOYSA-N
Formula:	C9H23N3
SMILES:	CN(C)CCN(C)CCN(C)C
Mol. weight [g/mol]:	173.30

Physical Properties

Property code	Value	Unit	Source
gf	357.24	kJ/mol	Joback Method
hf	-26.50	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	41.76	kJ/mol	Joback Method
log10ws	0.70		Crippen Method
logp	0.041		Crippen Method
mcvol	167.610	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	442.64	K	Joback Method
tc	602.08	K	Joback Method
tf	288.60	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.67	J/mol×K	602.08	Joback Method
cpg	444.36	J/mol×K	575.51	Joback Method
cpg	430.43	J/mol×K	548.93	Joback Method
cpg	415.84	J/mol×K	522.36	Joback Method
cpg	400.58	J/mol×K	495.79	Joback Method
cpg	384.62	J/mol×K	469.21	Joback Method

cpg	367.95	J/mol×K	442.64	Joback Method
pvap	1.34	kPa	353.07	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	0.44	kPa	333.14	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	0.79	kPa	343.19	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	1.33	kPa	353.06	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	0.24	kPa	323.03	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	2.17	kPa	362.82	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	2.18	kPa	362.92	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	2.18	kPa	362.95	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	0.24	kPa	323.03	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	0.24	kPa	323.03	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	0.12	kPa	312.88	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	0.06	kPa	303.05	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	0.06	kPa	303.05	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	0.03	kPa	292.98	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	0.03	kPa	292.98	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}

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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'',N''-pentamethyldiethylenetriamine (PMDETA)) + water}:	https://www.doi.org/10.1016/j.jct.2018.08.025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume