

1,3-Propanediamine, N,N,N',N'-tetramethyl-

Other names:	(CH3)2N(CH2)3N(CH3)2 1,3-Bis(dimethylamino)propane Bis[(dimethylamino)methyl]methane N,N,N',N'-Tetramethyl-1,3-diaminopropane N,N,N',N'-Tetramethyl-1,3-propanediamine N,N,N',N'-Tetramethyltrimethylenediamine Propane-1,3-diamine, N,N,N',N'-tetramethyl- Tetramethylpropanediamine Tetramethyltrimethylenediamine
Inchi:	InChI=1S/C7H18N2/c1-8(2)6-5-7-9(3)4/h5-7H2,1-4H3
InchiKey:	DMQSHEKGGUOYJS-UHFFFAOYSA-N
Formula:	C7H18N2
SMILES:	CN(C)CCCN(C)C
Mol. weight [g/mol]:	130.23
CAS:	110-95-2

Physical Properties

Property code	Value	Unit	Source
affp	1035.20	kJ/mol	NIST Webbook
basg	985.40	kJ/mol	NIST Webbook
gf	229.62	kJ/mol	Joback Method
hf	-52.75	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	35.26	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.84	eV	NIST Webbook
log10ws	0.11		Crippen Method
logp	0.500		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	417.20	K	NIST Webbook
tb	418.70	K	NIST Webbook
tc	545.94	K	Joback Method
tf	191.20 ± 0.60	K	NIST Webbook
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.85	J/mol×K	384.44	Joback Method
cpg	314.62	J/mol×K	519.02	Joback Method
cpg	302.76	J/mol×K	492.11	Joback Method
cpg	290.37	J/mol×K	465.19	Joback Method
cpg	277.44	J/mol×K	438.27	Joback Method
cpg	263.93	J/mol×K	411.36	Joback Method
cpg	325.97	J/mol×K	545.94	Joback Method
hvapt	45.30	kJ/mol	298.15	Vapor pressure and enthalpy of vaporization of aliphatic propanediamines
rho1	761.40	kg/m3	323.15	Mutual diffusion coefficients, density, and viscosity of aqueoussolutions of new polyamine CO2absorbents
rho1	765.00	kg/m3	318.15	Mutual diffusion coefficients, density, and viscosity of aqueoussolutions of new polyamine CO2absorbents
rho1	767.40	kg/m3	313.15	Mutual diffusion coefficients, density, and viscosity of aqueoussolutions of new polyamine CO2absorbents
rho1	770.90	kg/m3	308.15	Mutual diffusion coefficients, density, and viscosity of aqueoussolutions of new polyamine CO2absorbents
rho1	774.80	kg/m3	303.15	Mutual diffusion coefficients, density, and viscosity of aqueoussolutions of new polyamine CO2absorbents

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54936e+01
Coeff. B	-3.93231e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	302.05
Temperature range (K), max.	443.31

Sources

Mutual diffusion coefficients, density, and viscosity of aqueous solutions of several organic CO₂ absorbents: Crippen Method

<https://www.doi.org/10.1016/j.fluid.2013.11.028>

Joback Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

CO₂ Solubility Measurements and Modeling for Tertiary Diamines: Crippen Method:

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

<https://www.doi.org/10.1021/je500927h>

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

Vapor pressure and enthalpy of vaporization of aliphatic prepared diamines: McGowan Method:

<https://www.doi.org/10.1016/j.jct.2011.11.004>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C110952&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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