

1-Propanol, 3-(dimethylamino)-

Other names:	1-(Dimethylamino)propan-3-ol
	1-Dimethylamino-3-propanol
	3-(Dimethylamino)propanol
	3-(Dimethylamino)-1-propanol
	3-(Dimethylamino)propanol
	3-(N,N-Dimethylamino)-1-propanol
	3-(N,N-Dimethylamino)propanol
	3-(dimethylamino)propan-1-ol
	3-dimethylamino-1-propanol
	3-dimethylaminopropan-1-ol
	Dimethylaminopropanol
	Dimethylpropanolamine
	N,N-Dimethyl-3-hydroxypropylamine
	N,N-Dimethyl-«gamma»-aminopropanol
	N,N-Dimethyl-Â«gammaÂ»-aminopropanol
	N,N-Dimethylaminopropanol
	N,N-Dimethylpropanolamine
	NSC 62086
	«gamma»-(Dimethylamino)propanol
	Â«gammaÂ»-(Dimethylamino)propanol
Inchi:	InChI=1S/C5H13NO/c1-6(2)4-3-5-7/h7H,3-5H2,1-2H3
InchiKey:	PYSGFFTXMUWEOT-UHFFFAOYSA-N
Formula:	C5H13NO
SMILES:	CN(C)CCCO
Mol. weight [g/mol]:	103.16
CAS:	3179-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.82	kJ/mol	Joback Method
hf	-231.23	kJ/mol	Joback Method
hfus	15.81	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
ie	8.74 ± 0.04	eV	NIST Webbook
log10ws	0.25		Crippen Method
logp	-0.070		Crippen Method
mcvol	97.160	ml/mol	McGowan Method

pc	3867.48	kPa	Joback Method
tb	436.70	K	NIST Webbook
tb	436.50 ± 0.50	K	NIST Webbook
tc	578.89	K	Joback Method
tf	239.40	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.87	J/mol×K	418.42	Joback Method
cpg	207.30	J/mol×K	445.16	Joback Method
cpg	216.34	J/mol×K	471.91	Joback Method
cpg	225.02	J/mol×K	498.65	Joback Method
cpg	233.35	J/mol×K	525.40	Joback Method
cpg	241.33	J/mol×K	552.14	Joback Method
cpg	248.97	J/mol×K	578.89	Joback Method
pvap	0.02	kPa	293.14	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	7.00e-03	kPa	283.15	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures

pvap	0.03	kPa	303.09	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	0.07	kPa	313.08	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	0.14	kPa	323.28	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	0.26	kPa	333.12	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	0.47	kPa	343.12	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures

pvap	1.42	kPa	363.17	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
pvap	2.31	kPa	373.10	Investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methyl-1-propanol (AMP), N-benzylethanolamine, or 3-dimethylamino-1-propanol solutions at several temperatures
rhoI	881.00	kg/m3	298.15	Volumetric, acoustic and transport properties of mixtures containing dimethyl sulfoxide and some amines or alkanolamines: Measurement and correlation
rhoI	883.00	kg/m3	298.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	879.10	kg/m3	303.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	875.10	kg/m3	308.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K

rhoI	886.70	kg/m3	293.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	867.20	kg/m3	318.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	863.10	kg/m3	323.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	859.10	kg/m3	328.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	855.00	kg/m3	333.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	850.80	kg/m3	338.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	846.70	kg/m3	343.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	885.00	kg/m3	293.15	Volumetric, acoustic and transport properties of mixtures containing dimethyl sulfoxide and some amines or alkanolamines: Measurement and correlation

rhoI	877.00	kg/m3	303.15	Volumetric, acoustic and transport properties of mixtures containing dimethyl sulfoxide and some amines or alkanolamines: Measurement and correlation
rhoI	869.00	kg/m3	313.15	Volumetric, acoustic and transport properties of mixtures containing dimethyl sulfoxide and some amines or alkanolamines: Measurement and correlation
rhoI	860.00	kg/m3	323.15	Volumetric, acoustic and transport properties of mixtures containing dimethyl sulfoxide and some amines or alkanolamines: Measurement and correlation
rhoI	871.20	kg/m3	313.15	Densities of unloaded and CO2-loaded 3-dimethylamino-1-propanol at temperatures (293.15 to 343.15) K
rhoI	880.82	kg/m3	298.15	Density, Speed of Sound, Viscosity and Surface Tension of 3-Dimethylamino-1-propylamine + Water, 3-Amino-1-propanol + 3-Dimethylamino-1-propanol, and (3-Amino-1-propanol + 3-Dimethylamino-1-propanol) + Water from T = (293.15 to 323.15) K

srf	0.03	N/m	298.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K
srf	0.03	N/m	303.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K
srf	0.03	N/m	308.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K
srf	0.03	N/m	313.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K
srf	0.03	N/m	318.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K

srf	0.03	N/m	323.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K
srf	0.03	N/m	333.15	Volumetric Properties, Viscosities, Refractive Indices and Surface Tensions for Aqueous N, ndimethylpropanolamine (DMPA) Solutions From 298.15 K to 343.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	352.30	K	4.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	352.90	K	4.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	368.30	K	9.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture

tbp	378.50	K	14.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	378.50	K	14.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	385.80	K	19.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	396.80	K	29.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	405.00	K	39.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	411.60	K	49.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture
tbp	417.20	K	59.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methyamino)propylamine, for post-combustion CO2 capture

tbp	421.70	K	69.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methlamino)propylamine, for post-combustion CO2 capture
tbp	426.30	K	79.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methlamino)propylamine, for post-combustion CO2 capture
tbp	429.90	K	89.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methlamino)propylamine, for post-combustion CO2 capture
tbp	433.70	K	99.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methlamino)propylamine, for post-combustion CO2 capture
tbrp	347.50 ± 1.50	K	4.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35176e+01
Coeff. B	-3.59566e+03
Coeff. C	-6.25390e+01
Temperature range (K), min.	302.99
Temperature range (K), max.	500.71

Sources

Volumetric Properties, Viscosities, Refractive Indices and Surface Tension of Propan-1-ol and CO ₂ removal efficiency in trans-oxirane (using 2,2,6,6-tetramethylpiperidine-1-oxyl) and 2,2,6,6-tetramethylpiperidine-1-oxyl	https://www.doi.org/10.1016/j.tca.2012.05.025
Surface tension of propan-1-ol aqueous solutions	https://www.doi.org/10.1016/j.jct.2019.07.004
3-Dimethylamino-1-propanol tertiary amine solutions: Equilibrium solubility and McGowan Method modeling	https://www.doi.org/10.1021/acs.jced.7b00042
(3-Amino-1-propanol + 3-Dimethylamino-1-propanol) + Water	https://www.doi.org/10.1016/j.jct.2018.03.020
Properties of mixtures containing dimethyl carbonate and some amines or alkanolamines: Measurement and investigation of the isothermal (vapour + liquid) equilibria of aqueous 2-amino-2-methylpropan-1-ol, 3-dimethylamino-1-propanol, or 3-dimethylamino-1-propanol + 2-(ethylamino)ethanol blended aqueous solutions	http://link.springer.com/article/10.1007/BF02311772
Excess molar enthalpies for binary mixtures of different amines with water: Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-dimethylamino-1-propanol, for post-combustion CO ₂ capture: Densities of unloaded and CO ₂ -loaded 3-dimethylamino-1-propanol at temperatures (299.15 to 323.15) K: Pressure: Crippen Method:	https://www.doi.org/10.1016/j.jct.2018.02.018
	https://www.chemeo.com/doc/models/crippen_log10ws
	https://www.doi.org/10.1016/j.jct.2010.04.015
	https://www.doi.org/10.1016/j.jct.2019.02.023
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3179633&Units=SI
	https://www.doi.org/10.1016/j.jct.2015.04.030
	https://www.doi.org/10.1016/j.jct.2019.06.017
	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1016/j.jct.2016.02.007
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp _g :	Ideal gas heat capacity
g _f :	Standard Gibbs free energy of formation
h _f :	Enthalpy of formation at standard conditions
h _{fus} :	Enthalpy of fusion at standard conditions
h _{vap} :	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log _{10ws} :	Log10 of Water solubility in mol/l
log _p :	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ρ _l :	Liquid Density
σ:	Surface Tension
t _b :	Normal Boiling Point Temperature
t _{bp} :	Boiling point at given pressure
t _{brp} :	Boiling point at reduced pressure
t _c :	Critical Temperature
t _f :	Normal melting (fusion) point

vc: Critical Volume

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