

Diethanolamine

Other names:	2,2'-Dihydroxydiethylamine
	2,2'-IMINOBIS-ETHANOL
	2,2'-Iminobis[ethanol]
	2,2'-Iminodi-1-ethanol
	2,2'-Iminodiethanol
	2,2'-azanediylbis(ethan-1-ol)
	2-[(2-Hydroxyethyl)amino]ethanol
	Bis(2-hydroxyethyl)amine
	Bis(hydroxyethyl)amine
	DEA
	DIETHYLOLAMINE
	Dabco DEOA-LF
	Di(2-hydroxyethyl)amine
	Diaethanolamin
	Diethanol, 2,2'-imino-
	Diethanolamin
	Diethylamine, 2,2'-dihydroxy-
	Diolamine
	Ethanol, 2,2'-iminobis-
	Ethanol, 2,2'-iminodi-
	Iminodiethanol
	N,N'-Iminodiethanol
	N,N-Bis(2-hydroxyethyl)amine
	N,N-Diethanolamine
	NCI-C55174
	NSC 4959
	Niax DEOA-LF
Inchi:	InChI=1S/C4H11NO2/c6-3-1-5-2-4-7/h5-7H,1-4H2
InchiKey:	ZBCBWPMODOFKDW-UHFFFAOYSA-N
Formula:	C4H11NO2
SMILES:	OCCNCCO
Mol. weight [g/mol]:	105.14
CAS:	111-42-2

Physical Properties

Property code	Value	Unit	Source
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affp	953.00	kJ/mol	NIST Webbook
basg	920.00	kJ/mol	NIST Webbook
chs	-2652.30 ± 2.50	kJ/mol	NIST Webbook
dvisc	0.5665700	Paxs	Densities, Viscosities, and Refractive Indices of Aqueous Alkanolamine Solutions as Potential Carbon Dioxide Removal Reagents
gf	-201.45	kJ/mol	Joback Method
hf	-397.10 ± 2.90	kJ/mol	NIST Webbook
hfs	-493.80 ± 2.60	kJ/mol	NIST Webbook
hfus	19.39	kJ/mol	Joback Method
hsub	96.70 ± 1.20	kJ/mol	NIST Webbook
hsub	105.90 ± 2.00	kJ/mol	NIST Webbook
hvap	64.29	kJ/mol	Joback Method
log10ws	0.79		Crippen Method
logp	-1.439		Crippen Method
mcvol	88.940	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	5065.79	kPa	Joback Method
ripol	2180.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	542.46	K	Experimental and predicted vapor-liquid equilibrium for binary systems with diethanolamine, m-cresol and p-cresol at 20.0 kPa
tb	544.20	K	NIST Webbook
tb	541.55	K	NIST Webbook
tc	687.52	K	Joback Method
tf	301.20 ± 0.60	K	NIST Webbook
tf	301.10 ± 0.07	K	NIST Webbook
tf	301.15	K	NIST Webbook
tf	300.15	K	Thermodynamic and Kinetic Studies of CO2 Capture by Glycol and Amine-Based Deep Eutectic Solvents
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.16	J/molxK	606.48	Joback Method
cpg	238.34	J/molxK	633.49	Joback Method
cpg	212.00	J/molxK	525.45	Joback Method
cpg	219.00	J/molxK	552.46	Joback Method
cpg	225.71	J/molxK	579.47	Joback Method
cpg	249.93	J/molxK	687.52	Joback Method
cpg	244.26	J/molxK	660.50	Joback Method
cps	137.00	J/molxK	298.15	NIST Webbook
dvisc	0.0025220	Paxs	423.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0148080	Paxs	363.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.1835000	Paxs	313.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K

dvisc	0.0104110	Paxs	373.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0080110	Paxs	383.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0231350	Paxs	353.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0337900	Paxs	343.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0036090	Paxs	413.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K

dvisc	0.0613600	Paxs	333.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.1006000	Paxs	323.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0059850	Paxs	393.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.3805000	Paxs	303.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
dvisc	0.0045840	Paxs	403.15	Viscometric and volumetric behaviour of binary mixtures of sulfolane and N-methylpyrrolidone with monoethanolamine and diethanolamine in the range 303 373 K
hvapt	74.40	kJ/mol	482.50	NIST Webbook
hvapt	77.00	kJ/mol	415.00	NIST Webbook
hvapt	70.60	kJ/mol	490.00	NIST Webbook

hvapt	69.00	kJ/mol	522.50	NIST Webbook
pvap	4.94	kPa	452.40	Vapor Pressures of Several Commercially Used Alkanolamines
pvap	1.44	kPa	427.50	Vapor Pressures of Several Commercially Used Alkanolamines
pvap	1.94	kPa	433.00	Vapor Pressures of Several Commercially Used Alkanolamines
pvap	2.94	kPa	441.40	Vapor Pressures of Several Commercially Used Alkanolamines
pvap	3.94	kPa	447.40	Vapor Pressures of Several Commercially Used Alkanolamines
rho1	1087.51	kg/m3	308.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K
rho1	1080.86	kg/m3	318.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K

rhoI	1077.49	kg/m3	323.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K
rhoI	1096.10	kg/m3	293.15	Density and Viscosity for Binary Mixtures of Diethylene Glycol Monobutyl Ether with Monoethanolamine, Diethanolamine, and Triethanolamine from (293.15 to 333.15) K
rhoI	1089.80	kg/m3	303.15	Density and Viscosity for Binary Mixtures of Diethylene Glycol Monobutyl Ether with Monoethanolamine, Diethanolamine, and Triethanolamine from (293.15 to 333.15) K
rhoI	1083.70	kg/m3	313.15	Density and Viscosity for Binary Mixtures of Diethylene Glycol Monobutyl Ether with Monoethanolamine, Diethanolamine, and Triethanolamine from (293.15 to 333.15) K
rhoI	1077.40	kg/m3	323.15	Density and Viscosity for Binary Mixtures of Diethylene Glycol Monobutyl Ether with Monoethanolamine, Diethanolamine, and Triethanolamine from (293.15 to 333.15) K

rhoI	1097.61	kg/m3	293.15	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1091.17	kg/m3	303.15	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1084.60	kg/m3	313.15	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1071.11	kg/m3	333.14	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1064.25	kg/m3	343.14	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1057.31	kg/m3	353.14	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1070.70	kg/m3	333.15	Density and Viscosity for Binary Mixtures of Diethylene Glycol Monobutyl Ether with Monoethanolamine, Diethanolamine, and Triethanolamine from (293.15 to 333.15) K

rhoI	1050.24	kg/m3	363.15	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1097.40	kg/m3	293.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures
rhoI	1090.50	kg/m3	303.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures
rhoI	1083.90	kg/m3	313.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures
rhoI	1077.10	kg/m3	323.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures

rhoI	1070.30	kg/m3	333.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures
rhoI	1063.50	kg/m3	343.15	Volumetric and viscometric behaviour of the binary systems of N-methyldiethanolamine and diethanolamine with 1-butyl-3-methylimidazolium acetate at various temperatures
rhoI	1107.05	kg/m3	278.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
rhoI	1103.88	kg/m3	283.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K

rhoI	1097.51	kg/m3	293.15	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
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rhoI	1091.06	kg/m3	303.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
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rhoI	1084.49	kg/m3	313.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
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rhoI	1077.78	kg/m3	323.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
rhoI	1071.00	kg/m3	333.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
rhoI	1064.14	kg/m3	343.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K

rhoI	1060.68	kg/m3	348.14	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
rhoI	1056.83	kg/m3	353.15	Densities and Excess Molar Volumes for Binary Mixtures of Diethanolamine with Water, Methanol, Ethanol and Ternary Solutions of Diethanolamine + Water with Methanol, Ethanol at Atmospheric Pressure from 278.15 to 353.15 K
rhoI	1084.70	kg/m3	313.15	Density and Viscosity of Aqueous Blends of Three Alkanolamines: N-Methyldiethanolamine, Diethanolamine, and 2-Amino-2-methyl-1-propanol in the Range of (303 to 343) K
rhoI	1077.40	kg/m3	323.15	Density and Viscosity of Aqueous Blends of Three Alkanolamines: N-Methyldiethanolamine, Diethanolamine, and 2-Amino-2-methyl-1-propanol in the Range of (303 to 343) K

rhoI	1070.30	kg/m3	333.15	Density and Viscosities of Aqueous Blends of Three Alkanolamines: N-Methyldiethanolamine, Diethanolamine, and 2-Amino-2-methyl-1-propanol in the Range of (303 to 343) K
rhoI	1094.02	kg/m3	298.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K
rhoI	1090.79	kg/m3	303.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K
rhoI	1077.88	kg/m3	323.15	Volumetric properties of binary mixtures of dimethyl sulfoxide with amines from (293.15 to 363.15) K
rhoI	1084.20	kg/m3	313.15	Densities and Viscosities of Aqueous Ternary Mixtures of 2-(Methylamino)ethanol and 2-(Ethylamino)ethanol with Diethanolamine, Triethanolamine, N-Methyldiethanolamine, or 2-Amino-1-methyl-1-propanol from 298.15 to 323.15 K

speedsl	1673.76	m/s	318.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K
speedsl	1711.30	m/s	303.15	Density, Speed of Sound, Viscosity, Surface Tension, and Excess Volume of N-Ethyl-2-pyrrolidone + Ethanolamine (or Diethanolamine or Triethanolamine) from T = (293.15 to 323.15) K
speedsl	1685.90	m/s	313.15	Density, Speed of Sound, Viscosity, Surface Tension, and Excess Volume of N-Ethyl-2-pyrrolidone + Ethanolamine (or Diethanolamine or Triethanolamine) from T = (293.15 to 323.15) K
speedsl	1661.10	m/s	323.15	Density, Speed of Sound, Viscosity, Surface Tension, and Excess Volume of N-Ethyl-2-pyrrolidone + Ethanolamine (or Diethanolamine or Triethanolamine) from T = (293.15 to 323.15) K

speedsl	1736.54	m/s	293.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K
speedsl	1723.96	m/s	298.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K
speedsl	1711.55	m/s	303.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K

speedsl	1698.70	m/s	308.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K
speedsl	1686.13	m/s	313.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K
speedsl	1739.20	m/s	293.15	Density, Speed of Sound, Viscosity, Surface Tension, and Excess Volume of N-Ethyl-2-pyrrolidone + Ethanolamine (or Diethanolamine or Triethanolamine) from T = (293.15 to 323.15) K
speedsl	1660.36	m/s	323.15	Density, Speed of Sound, Isentropic Compressibility, and Excess Volume of Binary Mixtures of 1-Amino-2-propanol or 3-Amino-1-propanol with 2-Amino-2-methyl-1-propanol, Diethanolamine, or Triethanolamine from (293.15 to 323.15) K

srf	0.05	N/m	298.15	Density, speed of sound, viscosity, refractive index and surface tension of N-methyl-2-pyrrolidone + diethanolamine (or triethanolamine) from T = (293.15 to 323.15) K
srf	0.05	N/m	293.15	Density, speed of sound, viscosity, refractive index and surface tension of N-methyl-2-pyrrolidone + diethanolamine (or triethanolamine) from T = (293.15 to 323.15) K
srf	0.05	N/m	313.15	Density, speed of sound, viscosity, refractive index and surface tension of N-methyl-2-pyrrolidone + diethanolamine (or triethanolamine) from T = (293.15 to 323.15) K
srf	0.05	N/m	323.15	Density, speed of sound, viscosity, refractive index and surface tension of N-methyl-2-pyrrolidone + diethanolamine (or triethanolamine) from T = (293.15 to 323.15) K
srf	0.05	N/m	303.20	Investigation of surface tension and viscosity for aqueous solutions of MEA-MeOH and DEA-MeOH
srf	0.04	N/m	313.20	Investigation of surface tension and viscosity for aqueous solutions of MEA-MeOH and DEA-MeOH

srf	0.04	N/m	323.20	Investigation of surface tension and viscosity for aqueous solutions of MEA-MeOH and DEA-MeOH
srf	0.05	N/m	303.15	Density, speed of sound, viscosity, refractive index and surface tension of N-methyl-2-pyrrolidone + diethanolamine (or triethanolamine) from T = (293.15 to 323.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	490.20	K	20.00	NIST Webbook
tbrp	427.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.72949e+01
Coeff. B	-5.79247e+03
Coeff. C	-8.45980e+01
Temperature range (K), min.	425.18
Temperature range (K), max.	567.97

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.16769e+02
Coeff. B	-1.89915e+04
Coeff. C	-2.88239e+01

Coeff. D	1.48221e-05
Temperature range (K), min.	301.15
Temperature range (K), max.	542.15

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	1093.6
100.00	303.15	1090.4
100.00	308.15	1087.1
100.00	313.15	1083.8
100.00	318.15	1080.6
100.00	323.15	1077.4
100.00	328.15	1074.1
100.00	333.15	1070.8
100.00	338.15	1067.4
100.00	343.15	1064.0
100.00	348.15	1060.6
100.00	353.15	1057.2
100.00	358.15	1053.7
100.00	363.15	1050.1
700.00	373.15	1043.3
700.00	383.15	1035.5
700.00	393.15	1028.1
700.00	403.15	1020.5
700.00	413.15	1012.9
700.00	423.15	1004.8

Reference

<https://www.doi.org/10.1021/je300345m>

Sources

Density and Viscosity of Aqueous Blends of Three Alkanolamines: 2-Amino-2-methyl-1-propanol in the Range of (303 to 343) K:

Major Resources of Several Commonly Used Alkanolamines: Diethanolamine, and

<https://www.doi.org/10.1021/je050462y>

<https://www.doi.org/10.1021/je101259r>

Solubility of Ethane in Aqueous Solutions of Monoethanolamine and Details of Partially Carbonated Aqueous Diethanolamine and Methylolammonium and Refractive Indices of Aqueous Alkanolamine Gels and Saturated Carbon Dioxide Surfactant Region and Excess Volume Expansion of the Predicted Phase Equilibrium Diagrams for Ethanolamine and Diethanolamine and the Solubility of Ethane in Aqueous Solutions of Monoethanolamine and Diethanolamine Blends and Methylolammonium (MDEA) and Diethanolamine (DEA): 25% MDEA + 25% DEA and 30% MDEA + 20% DEA:

<https://www.doi.org/10.1016/j.jct.2013.09.001>
<https://www.doi.org/10.1016/j.jct.2015.04.030>
<https://www.doi.org/10.1016/j.jct.2007.03.010>
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<https://www.doi.org/10.1016/j.jct.2011.03.016>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C111422&Units=SI>
<https://www.doi.org/10.1021/je300345m>
<https://www.doi.org/10.1016/j.jct.2014.03.032>
<https://www.doi.org/10.1021/je020206a>
<https://www.doi.org/10.1016/j.fluid.2015.03.021>
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<https://www.doi.org/10.1021/je020048n>
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<https://www.doi.org/10.1021/je5002957>
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<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1320>
<https://www.doi.org/10.1021/je060108f>
<https://www.doi.org/10.1021/je4000372>
<https://www.doi.org/10.1021/je050463q>
<https://www.doi.org/10.1021/acs.jced.6b00862>
<https://www.doi.org/10.1016/j.jct.2014.06.017>
<https://www.doi.org/10.1016/j.jct.2017.08.024>
<https://www.doi.org/10.1021/je400340s>
<https://www.cheric.org/files/research/kdb/mol/mol1320.mol>
<https://www.doi.org/10.1021/je060031v>
<https://www.doi.org/10.1021/je300530z>
<https://www.doi.org/10.1021/je300938w>
<https://www.doi.org/10.1021/je301123j>
<https://www.doi.org/10.1016/j.jct.2018.09.002>
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Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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