Ethanamine, N-ethyl-

Other names:	(C2H5)2NH
	DEA
	DIETHAMINE
	DIETHYLAMINE
	Diaethylamin
	Dietilamina
	Dwuetyloamina
	N,N-DIETHYLAMINE
	N-Ethylethanamine
	UN 1154
Inchi:	InChI=1S/C4H11N/c1-3-5-4-2/h5H,3-4H2,1-2H3
InchiKey:	HPNMFZURTQLUMO-UHFFFAOYSA-N
Formula:	C4H11N
SMILES:	CCNCC
Mol. weight [g/mol]:	73.14
CAS:	109-89-7

Physical Properties

Property code	Value	Unit	Source
af	0.2910		KDB
affp	952.40	kJ/mol	NIST Webbook
basg	919.40	kJ/mol	NIST Webbook
chl	-3035.00	kJ/mol	NIST Webbook
dm	1.10	debye	KDB
gf	72.14	kJ/mol	KDB
gyrad	3.2500		KDB
hf	-72.43	kJ/mol	KDB
hf	-99.80	kJ/mol	NIST Webbook
hfl	-131.00	kJ/mol	NIST Webbook
hfus	11.21	kJ/mol	Joback Method
hvap	31.30 ± 0.10	kJ/mol	NIST Webbook
hvap	31.20 ± 0.10	kJ/mol	NIST Webbook
hvap	31.18 ± 0.06	kJ/mol	NIST Webbook
hvap	31.47	kJ/mol	NIST Webbook
hvap	32.70 ± 0.20	kJ/mol	NIST Webbook
ie	8.51	eV	NIST Webbook
ie	8.01 ± 0.01	eV	NIST Webbook

ie	8.68	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
ie	8.63	eV	NIST Webbook
log10ws	-0.69		Crippen Method
logp	0.616		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
pc	3748.00 ± 100.00	kPa	NIST Webbook
pc	3747.98 ± 20.68	kPa	NIST Webbook
pc	3758.00	kPa	KDB
pc	3758.00 ± 15.00	kPa	NIST Webbook
pc	3758.00 ± 15.00	kPa	NIST Webbook
rhoc	242.81 ± 2.19	kg/m3	NIST Webbook
rinpol	556.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	548.90		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	560.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	546.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	548.90		NIST Webbook
rinpol	548.00		NIST Webbook
ripol	718.00		NIST Webbook
ripol	712.00		NIST Webbook
ripol	707.00		NIST Webbook
ripol	707.00		NIST Webbook
ripol	700.00		NIST Webbook
ripol	716.00		NIST Webbook
ripol	710.00		NIST Webbook
ripol	712.00		NIST Webbook

tb	328.67	K	Isobaric Vapor Liquid Equilibrium for the Binary Systems of Methanol, Diethylamine, and N,N-Diethylethanolamine at p = (60.0 and 101.3) kPa
tb	328.48 ± 0.15	K	NIST Webbook
tb	328.60	K	KDB
tb	329.45 ± 0.50	K	NIST Webbook
tb	328.65 ± 0.50	K	NIST Webbook
tb	329.10 ± 0.50	K	NIST Webbook
tb	329.05 ± 0.30	K	NIST Webbook
tb	328.65 ± 1.50	K	NIST Webbook
tb	328.15 ± 1.00	K	NIST Webbook
tb	328.45 ± 0.30	K	NIST Webbook
tb	328.65 ± 1.00	K	NIST Webbook
tb	328.65 ± 0.40	K	NIST Webbook
tb	328.55 ± 0.30	K	NIST Webbook
tb	328.65	K	NIST Webbook
tb	328.65 ± 0.60	K	NIST Webbook
tb	328.55 ± 0.40	K	NIST Webbook
tb	328.30	K	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
tb	328.48 ± 0.25	K	NIST Webbook
tb	328.70	K	NIST Webbook
tb	329.50	K	NIST Webbook
tb	328.20	K	NIST Webbook
tb	328.45	K	Study of a Binary Liquid Mixture of Diethylamine and 1-Decanol and Validation of Theoretical Approaches of Sound Speed at Different Temperatures
tb	328.65	K	Isobaric Vapor Liquid Equilibrium for the Binary Systems (Diethylamine + Ethanol), (Ethanol + N,N-Diethylethanolamine), and (Diethylamine + N,N-Diethylethanolamine) at p = (80.0 and 40.0) kPa
tb	329.65 ± 1.50	K	NIST Webbook
tc	496.50	K	NIST Webbook
tc	496.45 ± 0.50	K	NIST Webbook
tc	496.95 ± 0.30	K	NIST Webbook

tc	499.51 ± 0.30	K	NIST Webbook
tc	499.99 ± 0.20	K	NIST Webbook
tc	499.99 ± 0.20	K	NIST Webbook
tc	499.99	K	KDB
tc	499.50 ± 0.50	K	NIST Webbook
tf	223.15 ± 0.50	K	NIST Webbook
tf	223.15 ± 3.00	K	NIST Webbook
tf	225.15 ± 1.00	K	NIST Webbook
tf	223.15 ± 2.00	K	NIST Webbook
tf	223.35	K	NIST Webbook
tf	223.30	K	KDB
vc	0.301	m3/kmol	KDB
zc	0.2720980		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.62	J/mol×K	341.09	Joback Method
cpg	137.29	J/mol×K	369.47	Joback Method
cpg	145.65	J/mol×K	397.84	Joback Method
cpg	153.72	J/mol×K	426.22	Joback Method
cpg	161.49	J/mol×K	454.60	Joback Method
cpg	168.97	J/mol×K	482.97	Joback Method
cpg	176.17	J/mol×K	511.35	Joback Method
cpl	178.10	J/mol×K	298.15	NIST Webbook
cpl	178.10	J/mol×K	298.15	NIST Webbook
cpl	106.30	J/mol×K	290.00	NIST Webbook
hvapt	27.82	kJ/mol	329.20	KDB
hvapt	29.06	kJ/mol	328.70	NIST Webbook
hvapt	31.20	kJ/mol	315.00	NIST Webbook
hvapt	30.40	kJ/mol	381.00	NIST Webbook
hvapt	28.40	kJ/mol	463.50	NIST Webbook
hvapt	30.20 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	29.10 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	28.00 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	31.80	kJ/mol	302.50	NIST Webbook
hvapt	31.50	kJ/mol	313.50	NIST Webbook

pvap	101.30	kPa	328.67	Isobaric Vapor Liquid Equilibrium for the Binary Systems of Methanol, Diethylamine, and N,N-Diethylethanolamine at p = (60.0 and 101.3) kPa
pvap	86.66	kPa	323.90	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	66.66	kPa	316.70	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	101.33	kPa	328.30	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	33.33	kPa	299.50	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation

pvap	26.66	kPa	294.70	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
pvap	60.00	kPa	313.64	Isobaric Vapor Liquid Equilibrium for the Binary Systems of Methanol, Diethylamine, and N,N-Diethylethanolamine at p = (60.0 and 101.3) kPa
pvap	46.66	kPa	307.60	Evolution of the Liquid Vapor Equilibrium Properties of Several Unsymmetrical Amines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation
rhol	707.00	kg/m3	293.00	KDB
rhol	719.94	kg/m3	278.15	Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K
rhol	709.52	kg/m3	288.15	Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K
rhol	704.59	kg/m3	293.15	Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K
rhol	698.97	kg/m3	298.15	Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K

rhol	688.29	kg/m3	308.15	Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K
rhol	710.01	kg/m3	288.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa
rhol	672.10	kg/m3	323.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	699.33	kg/m3	298.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa
rhol	693.90	kg/m3	303.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa
rhol	704.80	kg/m3	293.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	699.30	kg/m3	298.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model

rhol	694.00	kg/m3	303.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	688.70	kg/m3	308.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	683.30	kg/m3	313.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	677.50	kg/m3	318.15	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model
rhol	704.78	kg/m3	293.15	Volumetric behaviour of binary mixtures of (trichloromethane + amines) at temperatures between T = (288.15 and 303.15) K at p = 0.1 MPa
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30719e+01
Coeff. B	-1.90734e+03
Coeff. C	-1.03073e+02
Temperature range (K), min.	252.27
Temperature range (K), max.	348.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.98569e+01
Coeff. B	-5.21958e+03
Coeff. C	-5.11442e+00
Coeff. D	2.34948e-06
Temperature range (K), min.	223.35
Temperature range (K), max.	496.60

Sources

KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1266
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1266
Isobaric Vapor Liquid Equilibrium for the Binary Systems (Diethylamine + Ethanol), (Ethanol + N,N-Diethylethanolamine), and (Diethylamine + N,N-Diethylethanolamine) at p = (80.0 and 101.3) kPa:	https://www.doi.org/10.1021/je4008712
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic study of heptane + amine mixtures. V. Excess and volumetric properties of binary mixtures of (trichloromethane + amines) at temperatures between T = 288.15 and 308.15 K at p = 0.1 MPa:	https://www.doi.org/10.1016/j.fluid.2014.12.017
Isobaric Binary Vapor Liquid Equilibrium Data at p = (80.0 and 101.3) kPa:	https://www.doi.org/10.1016/j.jct.2008.05.003
Study of a Binary Liquid Mixture of Diethylamine and 1-Decanol and Variation of Sound Speed at Different Temperatures:	https://www.doi.org/10.1021/je700619q
Validation of Theoretical Approaches of thermodynamic and transport properties of binary mixtures; friction theory (f-theory) and Joback method with PC-SAFT model:	https://www.doi.org/10.1016/j.jct.2015.04.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric study of diethylamine-water mixtures between 278.15 K and 308.15 K:	https://www.doi.org/10.1016/j.jct.2004.07.008
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Evolution of the Liquid Vapor Equilibrium Properties of Several Dialkylmethylamines: Determination of Their Binary Isobaric Diagrams and Applications to the Distillation:	https://www.doi.org/10.1021/je3009649
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1266
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Isobaric Vapor Liquid Equilibrium for the Binary Systems of Methanol, Diethylamine, and N,N-Diethylethanolamine at p = (60.0 and 101.3) kPa:	https://www.doi.org/10.1021/je301219c
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109897&Units=SI
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity

cpl:	Liquid phase heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter