1-Octanamine

Other names:	1-AMINOOCTANE
	1-Octylamine
	Amine 8D
	Armeen 8
	CAPRYLAMINE
	Caprylylamine
	Monoctylamine
	Monooctylamine
	NSC 9824
	Octanamine
	Octylamine
	n-C8H17NH2
	n-Octylamine
	n-Octylamine, mono-
Inchi:	InChI=1S/C8H19N/c1-2-3-4-5-6-7-8-9/h2-9H2,1H3
InchiKey:	IOQPZZOEVPZRBK-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCCCCCCN
Mol. weight [g/mol]:	129.24
CAS:	111-86-4

Physical Properties

Property code	Value	Unit	Source
affp	924.70	kJ/mol	NIST Webbook
affp	925.10	kJ/mol	NIST Webbook
affp	928.90	kJ/mol	NIST Webbook
basg	879.50 ± 9.20	kJ/mol	NIST Webbook
basg	895.00	kJ/mol	NIST Webbook
chl	-5635.38 ± 0.96	kJ/mol	NIST Webbook
gf	82.93	kJ/mol	Joback Method
hf	-173.50 ± 1.30	kJ/mol	NIST Webbook
hfl	-228.10 ± 1.20	kJ/mol	NIST Webbook
hfus	21.67	kJ/mol	Joback Method
hvap	54.60	kJ/mol	NIST Webbook
hvap	54.80 ± 0.50	kJ/mol	NIST Webbook
hvap	54.60	kJ/mol	NIST Webbook
hvap	54.63 ± 0.96	kJ/mol	NIST Webbook

ie	8.50	eV	NIST Webbook
log10ws	-2.75		Aqueous Solubility Prediction Method
logp	2.306		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2617.00 ± 400.00	kPa	NIST Webbook
rhoc	249.44 ± 29.73	kg/m3	NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1038.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1318.00		NIST Webbook
tb	452.75 ± 1.00	K	NIST Webbook
tb	452.80	K	NIST Webbook
tb	452.15 ± 1.00	K	NIST Webbook
tb	451.65 ± 3.00	K	NIST Webbook
tb	452.65 ± 3.00	K	NIST Webbook
tb	449.20	K	NIST Webbook
tb	459.15 ± 6.00	K	NIST Webbook
tb	452.00 ± 2.00	K	NIST Webbook
tb	445.65 ± 5.00	K	NIST Webbook
tc	641.00 ± 3.00	K	NIST Webbook
tf	272.90	K	Aqueous Solubility Prediction Method
tf	272.75 ± 0.20	K	NIST Webbook
tf	273.15 ± 0.50	K	NIST Webbook

tf	272.15 ± 0.50	K	NIST Webbook
vc	0.512	m3/kmol	Joback Method
volm	1.66e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.30	J/mol×K	514.07	Joback Method
cpg	292.59	J/mol×K	454.97	Joback Method
cpg	331.84	J/mol×K	543.62	Joback Method
cpg	343.86	J/mol×K	573.17	Joback Method
cpg	355.37	J/mol×K	602.72	Joback Method
cpg	366.38	J/mol×K	632.27	Joback Method
cpg	306.22	J/mol×K	484.52	Joback Method
cpl	309.30	J/mol×K	298.15	NIST Webbook
hvapt	50.80	kJ/mol	380.50	NIST Webbook
pvap	0.04	kPa	286.50	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.07	kPa	292.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

pvap	0.07	kPa	292.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.08	kPa	295.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.09	kPa	295.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.08	kPa	295.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.10	kPa	298.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.11	kPa	298.50	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.14	kPa	301.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.13	kPa	301.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.04	kPa	285.90	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.13	kPa	301.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.13	kPa	301.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.05	kPa	289.60	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

pvap	0.17	kPa	304.00	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.17	kPa	304.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.21	kPa	307.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.21	kPa	307.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.25	kPa	310.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.26	kPa	310.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.31	kPa	312.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.31	kPa	313.00	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.32	kPa	313.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.05	kPa	289.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.03	kPa	283.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.03	kPa	281.00	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.02	kPa	277.70	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.02	kPa	274.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.14	kPa	301.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.13	kPa	301.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.03	kPa	283.60	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
rhol	769.46	kg/m3	308.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations	
rhol	777.45	kg/m3	298.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations	
rhol	779.95	kg/m3	298.15	Experimental Solid + Liquid Equilibria and Excess Molar Volume of Alkanol + Octylamine Mixtures. Analysis in Terms of ERAS, DISQUAC, and Modified UNIFAC	

rhol	761.47	kg/m3	318.15	Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids with Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57539e+01
Coeff. B	-4.28704e+03
Coeff. C	-6.70140e+01
Temperature range (K), min.	344.20
Temperature range (K), max.	477.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.09173e+02
Coeff. B	-9.98021e+03
Coeff. C	-1.37762e+01
Coeff. D	8.43830e-06
Temperature range (K), min.	272.75
Temperature range (K), max.	627.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies.	https://www.doi.org/10.1016/j.fluid.2014.12.017
Experimental Solid + Liquid Equilibria and Excess Molar Volume of Alkanol + Octylamine Mixtures. Analysis in Terms of ERAS, DISQUAC, and Modified UNIFAC:	https://www.doi.org/10.1021/je0301895
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111864&Units=SI

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration:	https://www.doi.org/10.1021/je400212t
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1273.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1273
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Excess Molar Properties for Binary Systems of CnMIM-BF4 Ionic Liquids With Alkylamines in the Temperature Range (298.15 to 318.15) K. Experimental Results and Theoretical Model Calculations:	https://www.doi.org/10.1021/je301167q
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume

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