1-Propanamine, N,N-dipropyl-

Other names:	(n-C3H7)3N
	N,N-DIPROPYL-1-PROPYLAMINE
	N,N-Dipropyl-1-propanamine
	N,N-dipropylpropanamine
	Propyldi-n-propylamine
	TRIPROPYLAMINE
	Tri-n-propylamine
	UN 2260
	propanamine, N,N-dipropyl-
Inchi:	InChI=1S/C9H21N/c1-4-7-10(8-5-2)9-6-3/h4-9H2,1-3H3
InchiKey:	YFTHZRPMJXBUME-UHFFFAOYSA-N
Formula:	C9H21N
SMILES:	CCCN(CCC)CCC
Mol. weight [g/mol]:	143.27
CAS:	102-69-2

Physical Properties

Property code	Value	Unit	Source
affp	991.00	kJ/mol	NIST Webbook
basg	960.10	kJ/mol	NIST Webbook
chl	-6335.66 ± 0.79	kJ/mol	NIST Webbook
gf	135.68	kJ/mol	Joback Method
hf	-160.80 ± 0.80	kJ/mol	NIST Webbook
hfl	-206.90 ± 0.79	kJ/mol	NIST Webbook
hfus	22.09	kJ/mol	Joback Method
hvap	46.17	kJ/mol	NIST Webbook
hvap	46.15 ± 0.07	kJ/mol	NIST Webbook
hvap	46.20 ± 0.10	kJ/mol	NIST Webbook
ie	7.40	eV	NIST Webbook
ie	8.00 ± 0.30	eV	NIST Webbook
ie	7.03 ± 0.09	eV	NIST Webbook
ie	7.00 ± 0.10	eV	NIST Webbook
ie	7.23	eV	NIST Webbook
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	2.518		Crippen Method
mcvol	147.650	ml/mol	McGowan Method

pc	2302.53	kPa	Joback Method
rinpol	927.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	968.00		NIST Webbook
ripol	974.00		NIST Webbook
ripol	970.00		NIST Webbook
ripol	978.00		NIST Webbook
ripol	958.00		NIST Webbook
ripol	965.00		NIST Webbook
tb	429.65 ± 1.00	K	NIST Webbook
tb	429.15 ± 1.50	K	NIST Webbook
tb	427.65 ± 3.00	K	NIST Webbook
tb	427.65 ± 3.00	K	NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tb	429.15 ± 0.50	K	NIST Webbook
tb	429.15 ± 3.00	K	NIST Webbook
tb	429.65	K	KDB
tb	430.00 ± 4.00	K	NIST Webbook
tb	429.20	K	NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tb	427.40 ± 0.50	K	NIST Webbook
tc	579.60	K	Joback Method
tf	179.65	K	Aqueous Solubility Prediction Method
tf	172.65 ± 0.50	K	NIST Webbook
tf	179.65 ± 0.50	K	NIST Webbook
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.27	J/mol×K	579.60	Joback Method
cpg	303.35	J/mol×K	417.76	Joback Method
cpg	372.97	J/mol×K	552.63	Joback Method
cpg	360.15	J/mol×K	525.66	Joback Method
cpg	346.79	J/mol×K	498.68	Joback Method
cpg	332.88	J/mol×K	471.71	Joback Method
cpg	318.41	J/mol×K	444.73	Joback Method
dvisc	0.0005380	Pa×s	313.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
dvisc	0.0005980	Pa×s	303.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents
hvapt	45.60	kJ/mol	408.00	NIST Webbook
pvap	1.26	kPa	313.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
pvap	0.95	kPa	308.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15

pvap	0.28	kPa	288.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
pvap	0.20	kPa	283.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
pvap	0.71	kPa	303.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
pvap	0.52	kPa	298.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15

pvap	0.38	kPa	293.15	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
rhol	749.15	kg/m3	303.15	Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K
rhol	740.41	kg/m3	313.15	Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K
rhol	749.15	kg/m3	303.15	Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents III. Alkylamines in butanols 303.15K
rhol	752.10	kg/m3	298.15	Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57356e+01
Coeff. B	-4.09570e+03

Coeff. C	-6.05930e+01
Temperature range (K), min.	325.72
Temperature range (K), max.	453.50

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04659e+02
Coeff. B	-1.01020e+04
Coeff. C	-1.27761e+01
Coeff. D	5.18581e-06
Temperature range (K), min.	179.65
Temperature range (K), max.	577.50

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.33	0.0005977

Reference *https://www.doi.org/10.1016/j.tca.2009.07.008*

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1277.mol
Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions:	https://www.doi.org/10.1016/j.jct.2012.07.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents. IV. Alkylamines in 1,4-dioxane and dioxolane at 303.15K:	https://www.doi.org/10.1016/j.tca.2009.07.008
Thermodynamic study of (heptane + amine) mixtures. III. Excess and partial molar volumes of primary, secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102692&Units=SI
Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15:	https://www.doi.org/10.1021/je500358r
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents III. Alkylamines in butanols 303.15K:	https://www.doi.org/10.1016/j.tca.2009.02.005
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Studies of partial molar volumes of alkylamine in non-electrolyte solvents I. Alkylamines in hydrocarbons at 303.15 and 313.15K:	https://www.doi.org/10.1016/j.tca.2005.08.012
Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents: II. Haloalkanes and other polar solvents:	https://www.doi.org/10.1016/j.tca.2004.08.013
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1277

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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