Propylamine

Other names:	1-AMINOPROPANE
	1-Propanamine
	1-Propylamine
	MONOPROPYLAMINE
	Mono-n-propylamine
	NSC 7490
	PROPANAMINE
	Rcra waste number U194
	UN 1277
	n-C3H7NH2
	n-Propylamine
	propan-1-amine
Inchi:	InChI=1S/C3H9N/c1-2-3-4/h2-4H2,1H3
InchiKey:	WGYKZJWCGVVSQN-UHFFFAOYSA-N
Formula:	C3H9N
SMILES:	CCCN
Mol. weight [g/mol]:	59.11
CAS:	107-10-8

Physical Properties

Property code	Value	Unit	Source
af	0.3030		KDB
affp	907.50	kJ/mol	NIST Webbook
affp	917.80	kJ/mol	NIST Webbook
affp	907.10	kJ/mol	NIST Webbook
basg	883.90	kJ/mol	NIST Webbook
chl	-2344.00	kJ/mol	NIST Webbook
chl	-2365.00 ± 3.00	kJ/mol	NIST Webbook
dm	1.30	debye	KDB
gf	39.82	kJ/mol	KDB
hf	-72.43	kJ/mol	KDB
hf	-70.17 ± 0.54	kJ/mol	NIST Webbook
hf	-69.90 ± 0.80	kJ/mol	NIST Webbook
hf	-106.70	kJ/mol	NIST Webbook
hfl	-101.50 ± 0.40	kJ/mol	NIST Webbook
hfl	-138.00	kJ/mol	NIST Webbook
hfus	8.72	kJ/mol	Joback Method

hvap	31.43	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
hvap	29.20	kJ/mol	NIST Webbook
hvap	31.30	kJ/mol	NIST Webbook
hvap	31.30 ± 0.20	kJ/mol	NIST Webbook
ie	9.40 ± 0.30	eV	NIST Webbook
ie	8.78 ± 0.02	eV	NIST Webbook
ie	9.44	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.355		Crippen Method
mcvol	63.110	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
pc	4737.96 ± 101.32	kPa	NIST Webbook
pc	4720.00	kPa	KDB
pc	4737.96 ± 40.53	kPa	NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	472.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	515.00		NIST Webbook
ripol	816.00		NIST Webbook
ripol	787.00		NIST Webbook
ripol	785.00		NIST Webbook
ripol	817.00		NIST Webbook
ripol	815.00		NIST Webbook
ripol	783.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	816.00		NIST Webbook
sl	228.20	J/mol×K	NIST Webbook
sl	227.44	J/mol×K	NIST Webbook
tb	320.37	K	KDB

tc	497.00	K	NIST Webbook
tc	496.95 ± 1.50	K	NIST Webbook
tc	496.95 ± 0.50	K	NIST Webbook
tc	497.00	K	KDB
tc	499.20	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	190.00 ± 0.60	K	NIST Webbook
tf	190.00	K	KDB
tf	190.15	K	NIST Webbook
tf	190.15 ± 0.50	K	NIST Webbook
tt	188.36 ± 0.07	K	NIST Webbook
tt	188.36	K	KDB
tt	188.38 ± 0.01	K	NIST Webbook
vc	0.233	m3/kmol	KDB
volm	8.32e-05	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K
zc	0.2661370		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.30	J/mol×K	340.57	Joback Method
cpg	126.82	J/mol×K	431.57	Joback Method
cpg	133.15	J/mol×K	461.90	Joback Method
cpg	139.23	J/mol×K	492.23	Joback Method
cpg	145.07	J/mol×K	522.57	Joback Method
cpg	120.24	J/mol×K	401.24	Joback Method
cpg	113.40	J/mol×K	370.90	Joback Method
cpl	166.40	J/mol×K	298.15	NIST Webbook
cpl	162.30	J/mol×K	298.15	NIST Webbook
cpl	160.00	J/mol×K	298.15	NIST Webbook
cpl	162.51	J/mol×K	298.15	NIST Webbook

dvisc	0.0003851	Pa×s	288.15	Excess molar volume, viscosity, and refractive index study for the ternary mixture {2-methyl-2-butanol (1) + tetrahydrofuran (2) + propylamine (3)} at different temperatures. Application of the ERAS-model and Peng Robinson Stryjek Vera equation of state	
dvisc	0.0003585	Pa×s	298.15	Excess molar volume, viscosity, and refractive index study for the ternary mixture {2-methyl-2-butanol (1) + tetrahydrofuran (2) + propylamine (3)} at different temperatures. Application of the ERAS-model and Peng Robinson Stryjek Vera equation of state	
dvisc	0.0003530	Pa×s	303.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents	
dvisc	0.0003130	Pa×s	313.15	Studies of viscosities of dilute solutions of alkylamine in non-electrolyte solvents. II. Haloalkanes and other polar solvents	

dvisc	0.0003222	Pa×s	308.15	Excess molar volume, viscosity, and refractive index study for the ternary mixture {2-methyl-2-butanol (1) + tetrahydrofuran (2) + propylamine (3)} at different temperatures. Application of the ERAS-model and Peng Robinson Stryjek Vera equation of state
hfust	10.62	kJ/mol	188.36	NIST Webbook
hfust	10.97	kJ/mol	188.40	NIST Webbook
hfust	10.97	kJ/mol	188.36	NIST Webbook
hvapt	31.30	kJ/mol	323.00	NIST Webbook
hvapt	30.10	kJ/mol	313.00	NIST Webbook
hvapt	28.90	kJ/mol	328.00	NIST Webbook
hvapt	29.55	kJ/mol	320.40	NIST Webbook
hvapt	29.71	kJ/mol	322.20	KDB
rhol	712.25	kg/m3	298.15	Speeds of Sound and Isentropic Compressibilities of n-Alkoxyethanols and Polyethers with Propylamine at 298.15K
rhol	711.80	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives
rhol	716.48	kg/m3	293.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	696.04	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	712.76	kg/m3	298.15	Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K
rhol	706.10	kg/m3	303.15	Studies of viscosities of dilute solutions of alkylamines in non-electrolyte solvents III. Alkylamines in butanols 303.15K
rhol	705.88	kg/m3	303.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	711.21	kg/m3	298.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	717.00	kg/m3	293.00	KDB
rhol	700.62	kg/m3	308.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	706.10	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
sfust	56.40	J/mol×K	188.36	NIST Webbook
sfust	58.26	J/mol×K	188.36	NIST Webbook

speedsl	1217.97	m/s	298.15	Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K	
speedsl	1242.02	m/s	293.15	Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K	
speedsl	1266.07	m/s	288.15	Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K	
speedsl	1169.93	m/s	308.15	Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K	
speedsl	1193.96	m/s	303.15	Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K	
srf	0.02	N/m	293.20	KDB	

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.49672e+01
Coeff. B	-5.34711e+03
Coeff. C	-5.90378e+00
Coeff. D	3.59300e-06
Temperature range (K), min.	190.15
Temperature range (K), max.	496.95

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
303.15	101.33	0.0003527
Reference		*https://www.doi.org/10.1016/j.tca.2009.07.008*

Sources

Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K:	https://www.doi.org/10.1016/j.tca.2006.08.006
Speed of sound as a function of temperature and pressure for propane derivatives:	https://www.doi.org/10.1016/j.jct.2016.12.016
Studies of viscosities of dilute solutions of alkylamines in non electrolyte solvents: IV. Alkylamines in 1,4 dioxane and oxolane at 303.15K:	https://www.doi.org/10.1016/j.tca.2009.07.008
Mixing Properties for Binary Liquid Mixtures of Methyl tert-Butyl Ether with Propylamine and Dipropylamine at Temperatures from (288.15 to 308.15) K:	https://www.doi.org/10.1021/je900597n
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application to the ERAS model:	https://www.doi.org/10.1016/j.jct.2015.09.002
Excess molar volume, viscosity, and refractive index study for the ternary mixture (2-methyl-2-butanol (1) + acetylacetone (2) + propylamine (3)) at different temperatures. Application of the ERAS-model and Peng Robinson Stryjek Vera equation of state:	https://www.doi.org/10.1016/j.jct.2010.05.009
Thermodynamic study of (heptane + amine) mixtures (1). Excess and partial molar volumes:	https://www.doi.org/10.1016/j.jct.2010.12.025
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://www.doi.org/10.1016/j.fluid.2014.12.017
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1258.mol
Speeds of Sound and Isentropic Compressibilities of n-Alkoxyethanols and Dialkyl Ethers with Propylamine at 298.15K:	https://www.doi.org/10.1007/s10765-006-0047-0
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
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1258
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107108&Units=SI

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
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
hfust:	Enthalpy of fusion at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

volm:	Molar Volume
zc:	Critical Compressibility