Methane, nitro-

Other names:	CH3NO2
	NM
	NSC 428
	Nitrocarbol
	Nitrometan
	Nitromethane
	UN 1261
	nitromethane [NM]
Inchi:	InChI=1S/CH3NO2/c1-2(3)4/h1H3
InchiKey:	LYGJENNIWJXYER-UHFFFAOYSA-N
Formula:	CH3NO2
SMILES:	C[N+](=O)[O-]
Mol. weight [g/mol]:	61.04
CAS:	75-52-5

Physical Properties

Property code	Value	Unit	Source
af	0.3100		KDB
affp	754.60	kJ/mol	NIST Webbook
aigt	691.48	K	KDB
basg	721.60	kJ/mol	NIST Webbook
chl	-703.00 ± 1.00	kJ/mol	NIST Webbook
chl	-709.20	kJ/mol	NIST Webbook
chl	-709.15 ± 0.59	kJ/mol	NIST Webbook
chl	-733.25 ± 0.75	kJ/mol	NIST Webbook
chl	-709.60 ± 0.40	kJ/mol	NIST Webbook
dm	3.10	debye	KDB
ea	0.01	eV	NIST Webbook
ea	0.17 ± 0.01	eV	NIST Webbook
ea	0.44 ± 0.20	eV	NIST Webbook
ea	0.45 ± 0.05	eV	NIST Webbook
ea	0.96 ± 0.01	eV	NIST Webbook
ea	0.49 ± 0.11	eV	NIST Webbook
ea	0.50 ± 0.02	eV	NIST Webbook
ea	0.26 ± 0.08	eV	NIST Webbook
fll	7.30	% in Air	KDB
fpc	316.48	K	KDB

fpo	308.15	K	KDB
gf	-6.95	kJ/mol	KDB
gyrad	2.3060		KDB
hf	-81.00 ± 1.00	kJ/mol	NIST Webbook
hf	-74.78	kJ/mol	KDB
hfl	-113.00 ± 0.40	kJ/mol	NIST Webbook
hfl	-89.04 ± 0.75	kJ/mol	NIST Webbook
hfl	-113.10 ± 0.63	kJ/mol	NIST Webbook
hfus	9.71	kJ/mol	Joback Method
hvap	38.00 ± 0.40	kJ/mol	NIST Webbook
hvap	34.50 ± 0.08	kJ/mol	NIST Webbook
hvap	38.30 ± 0.10	kJ/mol	NIST Webbook
hvap	38.00 ± 0.40	kJ/mol	NIST Webbook
hvap	38.37	kJ/mol	NIST Webbook
hvap	37.20	kJ/mol	NIST Webbook
hvap	38.36	kJ/mol	NIST Webbook
ie	11.31 ± 0.01	eV	NIST Webbook
ie	11.23 ± 0.01	eV	NIST Webbook
ie	11.04 ± 0.02	eV	NIST Webbook
ie	11.12	eV	NIST Webbook
ie	11.07 ± 0.01	eV	NIST Webbook
ie	11.28 ± 0.08	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	11.13 ± 0.01	eV	NIST Webbook
ie	11.10 ± 0.05	eV	NIST Webbook
ie	11.07	eV	NIST Webbook
ie	11.08 ± 0.04	eV	NIST Webbook
ie	11.05	eV	NIST Webbook
ie	11.08 ± 0.03	eV	NIST Webbook
ie	11.29	eV	NIST Webbook
ie	11.47	eV	NIST Webbook
ie	11.31	eV	NIST Webbook
ie	11.80	eV	NIST Webbook
ie	11.29	eV	NIST Webbook
ie	11.10	eV	NIST Webbook
ie	11.28 ± 0.08	eV	NIST Webbook
ie	11.28	eV	NIST Webbook
log10ws	0.26		Estimated Solubility Method
log10ws	0.26		Aqueous Solubility Prediction Method
logp	-0.107		Crippen Method
mcvol	42.370	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB

nfpas	%!d(float64=4)		KDB
pc	5870.00 ± 58.65	kPa	NIST Webbook
pc	5870.00	kPa	KDB
pc	6310.00 ± 103.42	kPa	NIST Webbook
rhoc	352.20 ± 3.05	kg/m3	NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	526.13		NIST Webbook
rinpol	556.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	543.60		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	521.00		NIST Webbook
rinpol	487.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	565.00		NIST Webbook
rinpol	527.85		NIST Webbook
rinpol	528.16		NIST Webbook
rinpol	528.60		NIST Webbook
rinpol	531.15		NIST Webbook
rinpol	530.05		NIST Webbook
rinpol	529.26		NIST Webbook
rinpol	528.66		NIST Webbook
rinpol	528.15		NIST Webbook
rinpol	527.88		NIST Webbook
rinpol	527.75		NIST Webbook
rinpol	500.00		NIST Webbook
ripol	1188.50		NIST Webbook
ripol	1190.20		NIST Webbook
ripol	1178.50		NIST Webbook
ripol	1179.20		NIST Webbook
ripol	1180.60		NIST Webbook
ripol	1182.90		NIST Webbook
ripol	1184.70		NIST Webbook
ripol	1172.00		NIST Webbook

ripol	1159.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1187.80		NIST Webbook
ripol	1180.60		NIST Webbook
ripol	1187.80		NIST Webbook
ripol	1160.90		NIST Webbook
sl	171.75	J/mol×K	NIST Webbook
tb	373.35 ± 0.50	K	NIST Webbook
tb	374.34	K	KDB
tb	374.15 ± 2.00	K	NIST Webbook
tb	374.15 ± 1.00	K	NIST Webbook
tb	374.17 ± 0.30	K	NIST Webbook
tb	374.30 ± 0.50	K	NIST Webbook
tb	374.25 ± 0.30	K	NIST Webbook
tb	374.40 ± 0.50	K	NIST Webbook
tb	374.15 ± 1.50	K	NIST Webbook
tb	373.35 ± 0.50	K	NIST Webbook
tb	373.13 ± 0.07	K	NIST Webbook
tb	374.22 ± 0.08	K	NIST Webbook
tb	374.85 ± 0.30	K	NIST Webbook
tb	374.35 ± 0.05	K	NIST Webbook
tb	374.17 ± 0.25	K	NIST Webbook
tb	374.43 ± 0.30	K	NIST Webbook
tb	374.40	K	NIST Webbook
tb	374.40 ± 0.50	K	NIST Webbook
tc	588.00	K	NIST Webbook
tc	588.00	K	KDB
tc	588.00 ± 3.00	K	NIST Webbook
tf	244.32	K	Aqueous Solubility Prediction Method
tf	244.60 ± 0.05	K	NIST Webbook
tf	243.36	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
tf	244.60	K	KDB
tf	243.95 ± 0.30	K	NIST Webbook
tf	244.00 ± 2.00	K	NIST Webbook
tf	243.11 ± 0.05	K	NIST Webbook
tf	244.55 ± 0.40	K	NIST Webbook
tt	244.77 ± 0.02	K	NIST Webbook

vc	0.173	m3/kmol	KDB
zc	0.2077160		KDB
zra	0.23		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	71.78	J/mol×K	409.74	Joback Method
cpg	87.12	J/mol×K	552.22	Joback Method
cpg	83.59	J/mol×K	516.60	Joback Method
cpg	79.86	J/mol×K	480.98	Joback Method
cpg	75.92	J/mol×K	445.36	Joback Method
cpg	67.43	J/mol×K	374.12	Joback Method
cpg	90.47	J/mol×K	587.84	Joback Method
cpl	105.98	J/mol×K	298.15	NIST Webbook
cpl	106.22	J/mol×K	308.00	NIST Webbook
cpl	108.20	J/mol×K	313.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations
cpl	108.80	J/mol×K	313.00	NIST Webbook
cpl	108.60	J/mol×K	318.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations
cpl	107.30	J/mol×K	303.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations

cpl	106.90	J/mol×K	298.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations
cpl	106.60	J/mol×K	293.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations
cpl	100.00	J/mol×K	298.00	NIST Webbook
cpl	107.70	J/mol×K	308.15	Excess molar properties for binary systems of alkylimidazolium-based ionic liquids + nitromethane. Experimental results and ERAS-model calculations
hfust	9.70	kJ/mol	244.80	NIST Webbook
hfust	9.70	kJ/mol	244.77	NIST Webbook
hfust	9.70	kJ/mol	244.80	NIST Webbook
hvapt	38.27	kJ/mol	298.15	NIST Webbook
hvapt	34.41	kJ/mol	374.00	KDB
hvapt	35.20	kJ/mol	440.50	NIST Webbook
hvapt	35.20 ± 0.10	kJ/mol	353.00	NIST Webbook
hvapt	33.99	kJ/mol	374.40	NIST Webbook
hvapt	36.80	kJ/mol	369.00	NIST Webbook
hvapt	34.00 ± 0.10	kJ/mol	374.00	NIST Webbook
hvapt	37.20 ± 0.10	kJ/mol	318.00	NIST Webbook
hvapt	36.30 ± 0.10	kJ/mol	335.00	NIST Webbook
kvisc	0.0000005	m2/s	305.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution

kvisc	0.0000005	m2/s	308.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	
kvisc	0.0000005	m2/s	303.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	
kvisc	0.0000005	m2/s	300.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	
kvisc	0.0000006	m2/s	298.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	
kvisc	0.0000006	m2/s	295.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	

kvisc	0.0000006	m2/s	293.15	Densities, Viscosities, and Speeds of Sound of the Nitromethane + 1-Pentanol System near the Critical Demixing Temperature: Effect of Deuterium Substitution	
rfi	1.37956		298.15	Isothermal vapor liquid equilibria and excess Gibbs free energies in some binary nitroalkane + chloroalkane mixtures at temperatures from 298.15 K to 318.15 K	
rfi	1.37960		298.15	Density and refractive index in mixtures of ionic liquids and organic solvents: Correlations and predictions	
rfi	1.37930		298.15	Isothermal (vapour + liquid) equilibria for (nitromethane or nitroethane + 1,4-dichlorobutane) binary systems at temperatures between (343.15 and 363.15) K	
rfi	1.37940		298.15	Isothermal Vapor Liquid Equilibria for Nitromethane and Nitroethane + 1,3-Dichloropropane Binary Systems at Temperatures between (343.15 and 363.15) K	

rfi	1.37990		298.15	Physico-chemical studies of sodium tetraphenylborate and tetrabutylammonium tetraphenylborate in pure nitrobenzene and nitromethane and their binaries probed by conductometry, refractometry and FT-IR spectroscopy
rhol	1138.00	kg/m3	293.00	KDB
rhol	1103.79	kg/m3	318.15	Water as a solute in nitromethane: Effect of H2O-D2O isotope substitution on the solution volumetric properties between 278.15 K and 318.15 K
rhol	1131.10	kg/m3	298.15	Asymmetric liquid-liquid criticality in the ideal volumetric mixing approximation
rhol	1130.15	kg/m3	298.15	Exploration of Solvation Consequence of Ionic Liquid [Bu4PCH3SO3] in Various Solvent Systems by Conductance and FTIR Study
rhol	1130.90	kg/m3	298.15	Volumetric Properties for (Ionic Liquid + Methanol or Ethanol or 1-Propanol + Nitromethane) at 298.15 K and Atmospheric Pressure
rhol	1130.86	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K

rhol	1117.24	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1103.50	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1130.91	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1117.53	kg/m3	308.15	Water as a solute in nitromethane: Effect of H2O-D2O isotope substitution on the solution volumetric properties between 278.15 K and 318.15 K	
rhol	1103.55	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1130.90	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	

rhol	1117.28	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1103.53	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1130.95	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1117.32	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1103.57	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	
rhol	1130.76	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K	

rhol	1117.14	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1103.39	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1117.23	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1103.48	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	1131.18	kg/m3	298.15	Water as a solute in nitromethane: Effect of H2O-D2O isotope substitution on the solution volumetric properties between 278.15 K and 318.15 K
rhol	1133.40	kg/m3	298.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane

rhol	1126.60	kg/m3	303.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane
rhol	1119.70	kg/m3	308.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane
rhol	1112.90	kg/m3	313.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane
rhol	1106.00	kg/m3	318.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane
rhol	1144.75	kg/m3	288.15	Water as a solute in nitromethane: Effect of H2O-D2O isotope substitution on the solution volumetric properties between 278.15 K and 318.15 K

rhol	1158.25	kg/m3	278.15	Water as a solute in nitromethane: Effect of H2O-D2O isotope substitution on the solution volumetric properties between 278.15 K and 318.15 K
rhol	1130.15	kg/m3	298.15	Ionic solvation of tetrabutylammonium hexafluorophosphate in pure nitromethane, 1, 3-dioxolane and nitrobenzene: A comparative physicochemical study
rhol	1140.20	kg/m3	293.15	Density and Heat Capacity as a Function of Temperature for Binary Mixtures of 1-Butyl-3-methylpyridinium Tetrafluoroborate + Water, + Ethanol, and + Nitromethane
rhol	1117.29	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
sfust	39.64	J/mol×K	244.77	NIST Webbook
speedsl	1242.60	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories

speedsl	1282.03	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1321.74	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1242.76	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1282.12	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1321.50	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories

speedsl	1242.50	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1321.49	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1242.46	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1281.78	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	

speedsl	1321.20	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1321.33	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1242.39	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1281.77	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1321.26	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	

speedsl	1242.49	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1281.90	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1321.62	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	
speedsl	1242.47	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories	

speedsl	1281.75	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1321.16	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1242.45	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1281.87	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1321.18	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories

srf	0.04	N/m	293.20	KDB
svapt	128.36	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53705e+01
Coeff. B	-3.66507e+03
Coeff. C	-3.32310e+01
Temperature range (K), min.	244.60
Temperature range (K), max.	588.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.31812e+01
Coeff. B	-7.21717e+03
Coeff. C	-1.02078e+01
Coeff. D	8.36912e-06
Temperature range (K), min.	244.60
Temperature range (K), max.	588.15

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	1130.15

Reference *https://www.doi.org/10.1021/je400536f*

Sources

Density and refractive index in mixtures of ionic liquids and organic solvents: Correlations and predictions:	https://www.doi.org/10.1016/j.jct.2008.01.023
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Experimental and theoretical study of interaction between organic compounds and 1-(4-sulfobutyl)-3-methylimidazolium based ionic liquids:	https://www.doi.org/10.1016/j.fluid.2014.06.021
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
High-Pressure Vapor-Liquid Equilbria of Some Carbon Dioxide + Organic Binary Systems:	https://www.doi.org/10.1021/je0498560
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75525&Units=SI
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Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
ea:	Electron affinity
fll:	Lower Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
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
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
kvisc:	Kinematic viscosity
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
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
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
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter