Pyrrole

Other names:	1-Aza-2,4-cyclopentadiene
	1H-Pyrrole
	Azole
	Divinyleneimine
	Divinylenimine
	Imidole
	Monopyrrole
	NSC 62777
	Parzate
	Pyrrol
Inchi:	InChI=1S/C4H5N/c1-2-4-5-3-1/h1-5H
InchiKey:	KAESVJOAVNADME-UHFFFAOYSA-N
Formula:	C4H5N
SMILES:	c1cc[nH]c1
Mol. weight [g/mol]:	67.09
CAS:	109-97-7

Physical Properties

Property code	Value	Unit	Source
affp	875.40	kJ/mol	NIST Webbook
basg	843.80	kJ/mol	NIST Webbook
dm	1.80	debye	KDB
hf	143.20	kJ/mol	NIST Webbook
hf	108.30 ± 0.50	kJ/mol	NIST Webbook
hf	108.40	kJ/mol	KDB
hvap	45.20	kJ/mol	NIST Webbook
hvap	45.19	kJ/mol	NIST Webbook
hvap	45.37	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	41.80	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
ie	8.21 ± 0.00	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
ie	8.22 ± 0.05	eV	NIST Webbook

ie	8.10	eV	NIST Webbook
ie	8.21 ± 0.01	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
ie	8.21 ± 0.01	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	8.40 ± 0.05	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
log10ws	-0.17		Aqueous Solubility Prediction Method
logp	0.533		Crippen Method
mcvol	57.740	ml/mol	McGowan Method
pc	6340.00	kPa	KDB
pc	5674.20 ± 303.98	kPa	NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	758.00		NIST Webbook
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rinpol	762.00		NIST Webbook
rinpol	730.00		NIST Webbook
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rinpol	740.00	NIST Webbook
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rinpol	751.00	NIST Webbook
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rinpol	771.00	NIST Webbook
rinpol	757.00	NIST Webbook
rinpol	751.00	NIST Webbook
rinpol	752.00	NIST Webbook
ripol	1524.00	NIST Webbook
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ripol	1492.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1520.00	NIST Webbook
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ripol	1530.00	NIST Webbook
ripol	1490.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1472.00	NIST Webbook
ripol	1511.00	NIST Webbook
ripol	1508.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1532.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1514.00	NIST Webbook
ripol	1518.00	NIST Webbook
ripol	1507.00	NIST Webbook
ripol	1498.00	NIST Webbook
ripol	1505.00	NIST Webbook
ripol	1504.00	NIST Webbook
ripol	1509.00	NIST Webbook

ripol	1470.00		NIST Webbook
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ripol	1534.00		NIST Webbook
ripol	1488.00		NIST Webbook
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ripol	1545.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1498.00		NIST Webbook
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ripol	1512.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	403.20 ± 0.60	K	NIST Webbook
tb	402.85 ± 0.20	K	NIST Webbook
tb	402.50 ± 0.50	K	NIST Webbook
tb	402.95 ± 0.20	K	NIST Webbook

tb	403.65 ± 3.00	K	NIST Webbook
tb	403.15 ± 0.50	K	NIST Webbook
tb	403.15 ± 2.00	K	NIST Webbook
tb	403.20 ± 0.15	K	NIST Webbook
tb	402.95 ± 0.15	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tb	403.00 ± 2.00	K	NIST Webbook
tb	401.15 ± 1.50	K	NIST Webbook
tb	403.65 ± 1.50	K	NIST Webbook
tb	403.00	K	NIST Webbook
tb	403.70	K	NIST Webbook
tb	402.94	K	KDB
tc	639.70 ± 1.50	K	NIST Webbook
tc	625.15 ± 2.00	K	NIST Webbook
tc	639.80	K	NIST Webbook
tc	638.50	K	Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results
tc	639.70	K	KDB
tf	254.70 ± 0.50	K	NIST Webbook
tf	249.95	K	Aqueous Solubility Prediction Method
tf	249.73	K	KDB
tf	250.15 ± 0.60	K	NIST Webbook
tf	238.80 ± 0.40	K	NIST Webbook
tf	249.70 ± 0.20	K	NIST Webbook
tt	249.74	K	KDB
tt	249.74 ± 0.06	K	NIST Webbook
tt	249.74 ± 0.03	K	NIST Webbook
tt	249.73 ± 0.07	K	NIST Webbook
tt	249.74 ± 0.06	K	NIST Webbook
tt	249.75 ± 0.08	K	NIST Webbook
vc	0.200	m3/kmol	KDB
zc	0.2384000		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	7.91	kJ/mol	249.70	NIST Webbook
hfust	7.91	kJ/mol	249.70	NIST Webbook

hfust	7.91	kJ/mol	249.74	NIST Webbook
hvapt	42.50	kJ/mol	389.00	NIST Webbook
hvapt	42.50	kJ/mol	307.00	NIST Webbook
hvapt	38.75	kJ/mol	403.00	NIST Webbook
hvapt	41.90	kJ/mol	353.00	NIST Webbook
hvapt	41.90	kJ/mol	343.00	NIST Webbook
rfi	1.51030		293.20	Vapor Liquid Equilibrium Data for Binary Systems of 1H-Pyrrole with Butan-1-ol, Propan-1-ol, or Pentan-1-ol
rhol	967.00	kg/m3	294.00	KDB
rhol	965.90	kg/m3	298.15	(Liquid + Liquid) Equilibrium for (N,N-Dimethylformamide (DMF) + Hexadecane) at Temperatures between (293.15 and 313.15) K and Ternary Mixtures of (DMF + Hexadecane) with Either Quinoline, or Pyridine, or Pyrrole, or Aniline, or Indole at T = 298.15 K
rhol	965.90	kg/m3	298.15	Binary Liquid-Liquid Equilibrium (LLE) for N-Methylformamide (NMF) + Hexadecane between (288.15 and 318.15) K and Ternary LLE for Systems of NMF + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K

rhol	965.95	kg/m3	298.15	Liquid-Liquid Equilibria for Binary System of Ethanol + Hexadecane at Elevated Temperature and the Ternary Systems of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K
rhol	930.13	kg/m3	338.15	Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling
rhol	939.14	kg/m3	328.15	Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling
rhol	948.03	kg/m3	318.15	Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling
rhol	956.83	kg/m3	308.15	Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling
rhol	965.54	kg/m3	298.15	Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling
sfust	31.66	J/mol×K	249.74	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45716e+01
Coeff. B	-3.34243e+03
Coeff. C	-6.71870e+01
Temperature range (K), min.	301.19
Temperature range (K), max.	639.75

Sources

Liquid-Liquid Equilibria for Binary System of Ethanol + Hexadecane at Elevated Temperature and the Ternary System of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K:	https://www.doi.org/10.1021/je700233p
High pressure phase equilibria in the carbon dioxide + pyrrole system:	https://www.doi.org/10.1016/j.fluid.2008.09.019
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
(Liquid + Liquid) Equilibrium for (N,N-Dimethylformamide (DMF) + Hexadecane) at Temperatures between (293.15 and 313.15) K and Ternary Mixtures of (DMF + Hexadecane) with Either Quinoline, or Pyridine, or Pyrrole, or Aniline, or Indole at T = 298.15 K:	https://www.doi.org/10.1021/je9006234
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109977&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1338
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Binary Liquid-Liquid Equilibrium (LLE) for N-Methylformamide (NMF) + Hexadecane between (298.15 and 318.15) K and Ternary LLE for Systems of NMF + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K: Experiments, COSMO-RS prediction and NRTL correlation:	https://www.doi.org/10.1021/je8006265
Extraction of nitrogen compounds from diesel fuel using imidazolium and pyrrolidinium based ionic liquids: Liquid-Liquid Equilibrium Data of Ternary Systems of 1H-Pyrrole + Propan-1-ol, or Pentan-1-ol:	https://www.doi.org/10.1016/j.fluid.2015.07.021
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Phase equilibria and excess molar enthalpies study of the binary systems (pyrrole + hydrocarbon, or an alcohol) and modeling:	https://www.doi.org/10.1016/j.fluid.2013.10.029
Liquid-Liquid Equilibrium for Ternary Systems of N-Methylformamide + Pentane, + Hexane, + Heptane at 298.15 K:	https://www.doi.org/10.1021/acs.jced.9b00202
Phase Equilibrium Measurement and Correlation: Propan-1-ol, or Pentan-1-ol + Binary Systems of 1H-Pyrrole with 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results:	https://www.doi.org/10.1021/je3004194
Thermodynamic properties of pyrrole:	https://www.doi.org/10.1016/j.jct.2017.09.005

Legend

affp:	Proton affinity
basg:	Gas basicity
dm:	Dipole Moment
hf:	Enthalpy of formation 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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion 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

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