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	108.30 ± 0.50	kJ/mol	NIST Webbook
hf	108.40	kJ/mol	KDB
hf	143.20	kJ/mol	NIST Webbook
hvap	41.80	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
hvap	45.37	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	45.19	kJ/mol	NIST Webbook
ie	8.21 ± 0.00	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.22 ± 0.05	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.21	eV	NIST Webbook

ie	8.21 ± 0.01	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
ie	8.21 ± 0.01	eV	NIST Webbook
ie	8.40 ± 0.05	eV	NIST Webbook
ie	8.20 ± 0.01	eV	NIST Webbook
log10ws	-0.17		Aqueous Solubility Prediction Method
logp	0.533		Crippen Method
mcvol	57.740	ml/mol	McGowan Method
pc	5674.20 ± 303.98	kPa	NIST Webbook
pc	6340.00	kPa	KDB
rinpol	739.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	768.00		NIST Webbook
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rinpol	730.00		NIST Webbook
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rinpol	755.00		NIST Webbook
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rinpol	755.00		NIST Webbook
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rinpol	739.00	NIST Webbook
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rinpol	751.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	747.00	NIST Webbook
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rinpol	740.00	NIST Webbook
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ripol	1507.00	NIST Webbook
ripol	1498.00	NIST Webbook
ripol	1505.00	NIST Webbook
ripol	1509.00	NIST Webbook
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ripol	1534.00		NIST Webbook
ripol	1488.00		NIST Webbook
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ripol	1523.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1542.00		NIST Webbook
tb	402.94	K	KDB
tb	403.15 ± 2.00	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	403.20 ± 0.60	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	401.15 ± 1.50	K	NIST Webbook
tb	402.85 ± 0.20	K	NIST Webbook
tb	403.00 ± 2.00	K	NIST Webbook
tb	403.00	K	NIST Webbook
tb	403.70	K	NIST Webbook
tb	403.65 ± 1.50	K	NIST Webbook
tc	639.70	K	KDB
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 ± 1.50	K	NIST Webbook
tf	254.70 ± 0.50	K	NIST Webbook
tf	249.73	K	KDB
tf	249.95	K	Aqueous Solubility Prediction Method
tf	238.80 ± 0.40	K	NIST Webbook
tf	250.15 ± 0.60	K	NIST Webbook
tf	249.70 ± 0.20	K	NIST Webbook
tt	249.75 ± 0.08	K	NIST Webbook
tt	249.74	K	KDB
tt	249.73 ± 0.07	K	NIST Webbook
tt	249.74 ± 0.03	K	NIST Webbook
tt	249.74 ± 0.06	K	NIST Webbook
tt	249.74 ± 0.06	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	249.74	NIST Webbook
hfust	7.91	kJ/mol	249.70	NIST Webbook

hfust	7.91	kJ/mol	249.70	NIST Webbook
hvapt	42.50	kJ/mol	389.00	NIST Webbook
hvapt	38.75	kJ/mol	403.00	NIST Webbook
hvapt	42.50	kJ/mol	307.00	NIST Webbook
hvapt	41.90	kJ/mol	343.00	NIST Webbook
hvapt	41.90	kJ/mol	353.00	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	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	967.00	kg/m3	294.00	KDB
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
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	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	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	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	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	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
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

Vapor Liquid Equilibrium Data for Binary Systems of 1H-Pyrrole with Butan-1-ol, Propan-1-ol, or Pentan-1-ol:	https://www.doi.org/10.1021/je3004194
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:	https://www.doi.org/10.1021/je8006265
Extraction of nitrogen compounds from diesel fuel using imidazolium- and pyridinium-based ionic liquids: Experiments, COSMO-RS prediction and NRTL correlation:	https://www.doi.org/10.1016/j.fluid.2015.07.021
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid-Liquid Equilibrium for Ternary Systems of N-Methylformamide + Pyrrole/Indole + Alkanes at 298.15 K: Phase Equilibrium Measurement and Correlation:	https://www.doi.org/10.1021/acs.jced.9b00202
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:	https://www.doi.org/10.1021/je700233p
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
(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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
High-pressure phase equilibria in the carbon dioxide + pyrrole system:	https://www.doi.org/10.1016/j.fluid.2008.09.019
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1338
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results:	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