

Indole

Other names:	1-AZAINDENE 1-BENZAZOLE 1-H-indol 1-benzo[b]pyrrole 1H-Indole 2,3-Benzopyrrole Benzopyrrole Indol KETOLE
Inchi:	InChI=1S/C8H7N/c1-2-4-8-7(3-1)5-6-9-8/h1-6,9H
InchiKey:	SIKJAQJRHWYJAI-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	c1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	117.15
CAS:	120-72-9

Physical Properties

Property code	Value	Unit	Source
affp	933.40	kJ/mol	NIST Webbook
basg	901.90	kJ/mol	NIST Webbook
chs	-4265.20 ± 4.20	kJ/mol	NIST Webbook
chs	-4240.50	kJ/mol	NIST Webbook
chs	-4235.13 ± 0.63	kJ/mol	NIST Webbook
ea	0.00 ± 0.00	eV	NIST Webbook
hfs	86.65 ± 0.75	kJ/mol	NIST Webbook
hsub	77.60 ± 1.10	kJ/mol	NIST Webbook
hsub	95.00	kJ/mol	NIST Webbook
ie	7.92 ± 0.05	eV	NIST Webbook
ie	7.87	eV	NIST Webbook
ie	7.75 ± 0.01	eV	NIST Webbook
ie	7.76 ± 0.00	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
ie	7.75 ± 0.05	eV	NIST Webbook
ie	7.76 ± 0.00	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
ie	8.29 ± 0.05	eV	NIST Webbook
ie	7.90	eV	NIST Webbook

ie	7.76 ± 0.00	eV	NIST Webbook
log10ws	-1.52		Aqueous Solubility Prediction Method
log10ws	-1.52		Estimated Solubility Method
logp	1.686		Crippen Method
mcvol	94.640	ml/mol	McGowan Method
rinpol	1270.40		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1304.00		NIST Webbook
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ripol	2463.00		NIST Webbook
tb	527.20	K	NIST Webbook
tb	526.00 ± 4.00	K	NIST Webbook
tb	526.65 ± 0.70	K	NIST Webbook
tb	526.15 ± 0.60	K	NIST Webbook
tf	324.00 ± 3.00	K	NIST Webbook
tf	324.80 ± 0.60	K	NIST Webbook
tf	324.00 ± 2.00	K	NIST Webbook
tf	325.00 ± 2.00	K	NIST Webbook
tf	325.70 ± 2.00	K	NIST Webbook
tf	324.95 ± 0.05	K	NIST Webbook
tf	325.52	K	Solid-liquid equilibria of indole binary systems
tf	325.32	K	Aqueous Solubility Prediction Method
tf	325.65 ± 0.50	K	NIST Webbook
tf	325.00 ± 2.00	K	NIST Webbook
tf	325.65 ± 0.50	K	NIST Webbook
tf	325.00 ± 3.00	K	NIST Webbook
tf	326.25 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	78.40 ± 1.40	kJ/mol	283.00	NIST Webbook
hsubt	75.00	kJ/mol	305.00	NIST Webbook
hsubt	77.80 ± 1.60	kJ/mol	289.00	NIST Webbook
hsubt	70.00	kJ/mol	292.00	NIST Webbook
hsubt	74.90	kJ/mol	305.50	NIST Webbook
rho1	1216.68	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
rho5	1216.65	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
rho6	1216.68	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44186e+01
Coeff. B	-4.23985e+03
Coeff. C	-9.45730e+01
Temperature range (K), min.	394.61
Temperature range (K), max.	560.13

Datasets

Specific volume, m3/kg

Temperature, K - Liquid	Pressure, kPa - Liquid	Specific volume, m3/kg - Liquid
323.15	100.00	0.0009
333.15	100.00	0.0009
333.15	10000.00	0.0009
333.15	20000.00	0.0009
333.15	30000.00	0.0009
333.15	40000.00	0.0009
333.15	50000.00	0.0009
343.15	100.00	0.0009
343.15	10000.00	0.0009
343.15	20000.00	0.0009
343.15	30000.00	0.0009

343.15	40000.00	0.0009
343.15	50000.00	0.0009
343.15	60000.00	0.0009
343.15	70000.00	0.0009
343.15	80000.00	0.0009
353.15	100.00	0.0009
353.15	10000.00	0.0009
353.15	20000.00	0.0009
353.15	30000.00	0.0009
353.15	40000.00	0.0009
353.15	50000.00	0.0009
353.15	60000.00	0.0009
353.15	70000.00	0.0009
353.15	80000.00	0.0009
353.15	90000.00	0.0009
353.15	100000.00	0.0009
353.15	110000.00	0.0009

Reference

<https://www.doi.org/10.1007/s10765-009-0625-z>

Sources

McGowan Method:

Estimated Solubility Method:

(Liquid + Liquid) Equilibrium for (N,N-Dimethylformamide (DMF) + Hexadecane) at Temperatures between 343.15 and 353.15 K: Vapor Pressure of Indole and 2-Methylnaphthalene and Aqueous Solubility Reduction Method

370 K: N-Propylene, or Pyridine, or Pyrrole, or Aniline, or Indole at T = 298.15 K

Binary Liquid-Liquid Equilibrium (LLE) for N-Methylformamide (NMF) + Hexadecane between 288.15 and 343.15 K

Systems of N-Methylformamide Systems of N-Methylformamide + N-Propylene, or Pyridine, or Pyrrole, or Aniline, or Indole at T = 298.15 K

Phase Equilibrium Measurements: Correlation

Binary Liquid-Liquid Equilibrium for ternary mixtures of formamide (or ethylene glycol, or monoethanolamine) + indole + 2-methylnaphthalene at 343.15 K

System of Ethanol + Hexadecane at 343.15 K

NIST Webbook

Temperature and the Ternary Systems of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K:

<http://link.springer.com/article/10.1007/BF02311772>

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

<https://www.doi.org/10.1021/je9006234>

<https://www.doi.org/10.1007/s10765-009-0625-z>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<https://www.doi.org/10.1021/je8006265>

<https://www.doi.org/10.1021/acs.jced.9b00202>

<https://www.doi.org/10.1016/j.tca.2016.10.003>

<https://www.doi.org/10.1016/j.fluid.2015.04.001>

<https://www.cheric.org/files/research/kdb/mol/mol1478.mol>

<https://www.doi.org/10.1021/je700233p>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C120729&Units=SI>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rho:	Liquid Density
rhos:	Solid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point
vols:	Specific Volume

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