Isoquinoline

Other names:	2-Azanaphthalene
	2-Benzanine
	2-Benzazine
	BENZOPYRIDINE
	BETA-QUINOLINE
	Benzo[c]pyridine
	Isochinolin
	Leucoline
	NSC 3395
	«beta»-Quinoline
	Â«betaÂ»-Quinoline
Inchi:	InChI=1S/C9H7N/c1-2-4-9-7-10-6-5-8(9)3-1/h1-7H
InchiKey:	AWJUIBRHMBBTKR-UHFFFAOYSA-N
Formula:	C9H7N
SMILES:	c1ccc2cnccc2c1
Mol. weight [g/mol]:	129.16
CAS:	119-65-3

Physical Properties

Property code	Value	Unit	Source
affp	951.70	kJ/mol	NIST Webbook
basg	919.90	kJ/mol	NIST Webbook
chl	-4686.46 ± 0.75	kJ/mol	NIST Webbook
chl	-4686.46 ± 0.75	kJ/mol	NIST Webbook
hf	204.61	kJ/mol	NIST Webbook
hf	204.00	kJ/mol	NIST Webbook
hfl	145.10 ± 0.88	kJ/mol	NIST Webbook
hfl	144.50 ± 0.84	kJ/mol	NIST Webbook
hvap	59.50	kJ/mol	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.53 ± 0.02	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.53 ± 0.05	eV	NIST Webbook
ie	8.55 ± 0.02	eV	NIST Webbook

log10ws	-1.45		Aqueous Solubility Prediction Method
log10ws	-1.45		Estimated Solubility Method
logp	2.235		Crippen Method
mcvol	104.430	ml/mol	McGowan Method
pc	5100.00	kPa	KDB
rinpol	214.14		NIST Webbook
rinpol	212.10		NIST Webbook
rinpol	215.61		NIST Webbook
rinpol	214.14		NIST Webbook
rinpol	215.61		NIST Webbook
rinpol	214.41		NIST Webbook
rinpol	213.19		NIST Webbook
rinpol	214.68		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1272.90		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1272.90		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1241.60		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1225.20		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	212.10		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1958.00		NIST Webbook
sl	215.98	J/mol×K	NIST Webbook
ss	171.06	J/mol×K	NIST Webbook

tb	516.37	K	KDB
tc	803.00	K	KDB
tc	803.15 ± 7.50	K	NIST Webbook
tf	299.38	K	Aqueous Solubility Prediction Method
tf	299.62	K	KDB
tt	299.62 ± 0.03	K	NIST Webbook
vc	0.374	m3/kmol	KDB
zc	0.2856860		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	196.16	J/mol×K	298.15	NIST Webbook
cps	177.68	J/mol×K	298.15	NIST Webbook
hfust	13.54	kJ/mol	299.60	NIST Webbook
hfust	13.54	kJ/mol	299.60	NIST Webbook
hvapt	58.90 ± 0.10	kJ/mol	439.50	NIST Webbook
hvapt	56.40 ± 0.10	kJ/mol	439.50	NIST Webbook
hvapt	49.40 ± 0.20	kJ/mol	439.50	NIST Webbook
hvapt	47.00 ± 0.30	kJ/mol	439.50	NIST Webbook
hvapt	51.00	kJ/mol	478.00	NIST Webbook
hvapt	54.10 ± 0.10	kJ/mol	439.50	NIST Webbook
hvapt	51.70 ± 0.10	kJ/mol	439.50	NIST Webbook
rhol	1091.00	kg/m3	303.00	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	5.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47493e+01
Coeff. B	-4.49042e+03
Coeff. C	-7.17640e+01
Temperature range (K), min.	382.27
Temperature range (K), max.	547.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.36292e+01
Coeff. B	-9.42215e+03
Coeff. C	-8.23896e+00
Coeff. D	2.68300e-06
Temperature range (K), min.	299.45
Temperature range (K), max.	803.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1363.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C119653&Units=SI

Liquid-Liquid Equilibrium for the Ternary Systems (Methyl Isobutyl Ketone + Quinoline or Isoquinoline + Water) at 298.15, 318.15, and 338.15 K: https://www.doi.org/10.1021/acs.jced.8b00096

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1363

Legend

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

cpl: Liquid phase heat capacity

cps: Solid phase heat capacity

hf: Enthalpy of formation at standard conditions

hfl:	Liquid phase 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility