Quinoline

Other names:	1-Azanaphthalene
	1-Benzazine
	B 500
	BENZOPYRIDINE
	Benzo[b]Pyridine
	Chinoleine
	Chinolin
	Chinoline
	LEUCOL
	Leucoline
	Leukol
	NSC 3396
	Quinolin
	UN 2656
	USAF EK-218
Inchi:	InChI=1S/C9H7N/c1-2-6-9-8(4-1)5-3-7-10-9/h1-7H
InchiKey:	SMWDFEZZVXVKRB-UHFFFAOYSA-N
Formula:	C9H7N
SMILES:	c1ccc2ncccc2c1
Mol. weight [g/mol]:	129.16
CAS:	91-22-5

Physical Properties

Property code	Value	Unit	Source
affp	953.20	kJ/mol	NIST Webbook
aigt	753.15	K	KDB
basg	921.40	kJ/mol	NIST Webbook
chl	-4683.20 ± 0.80	kJ/mol	NIST Webbook
fpo	380.37	K	KDB
hf	200.52	kJ/mol	NIST Webbook
hfl	141.22 ± 0.92	kJ/mol	NIST Webbook
hvap	47.45	kJ/mol	NIST Webbook
hvap	59.31 ± 0.20	kJ/mol	NIST Webbook
hvap	58.10	kJ/mol	NIST Webbook
hvap	59.30	kJ/mol	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.62	eV	NIST Webbook

ie	8.62	eV	NIST Webbook
ie	8.63 ± 0.02	eV	NIST Webbook
ie	8.67 ± 0.05	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-1.30		Estimated Solubility Method
log10ws	-1.30		Aqueous Solubility Prediction Method
logp	2.235		Crippen Method
mcvol	104.430	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=2)		KDB
pc	5780.00 ± 303.98	kPa	NIST Webbook
pc	4860.00	kPa	KDB
rinpol	1247.00		NIST Webbook
rinpol	210.32		NIST Webbook
rinpol	210.26		NIST Webbook
rinpol	210.17		NIST Webbook
rinpol	210.26		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1247.70		NIST Webbook
rinpol	1221.60		NIST Webbook
rinpol	1224.70		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1237.40		NIST Webbook
rinpol	1203.70		NIST Webbook
rinpol	1224.70		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1237.40		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1230.00		NIST Webbook

rinpol	1200.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1240.30		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1221.60		NIST Webbook
rinpol	1221.60		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	210.70		NIST Webbook
rinpol	210.37		NIST Webbook
rinpol	206.00		NIST Webbook
rinpol	210.18		NIST Webbook
rinpol	209.51		NIST Webbook
rinpol	209.70		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1892.00		NIST Webbook
sl	217.10	J/mol×K	NIST Webbook
sl	219.69	J/mol×K	NIST Webbook
sl	219.72	J/mol×K	NIST Webbook
tb	510.31	K	KDB
tb	510.85	K	Vapor Pressures and Vapor-Liquid Equilibria of the 2,2,2-Trifluoroethanol + Quinoline System
tc	782.00	K	KDB
tc	782.15 ± 3.00	K	NIST Webbook
tc	800.15 ± 3.00	K	NIST Webbook

tc	793.55 ± 10.00	K	NIST Webbook
tf	258.26	K	Aqueous Solubility Prediction Method
tf	250.75 ± 0.60	K	NIST Webbook
tf	258.21 ± 0.25	K	NIST Webbook
tf	258.30 ± 0.15	K	NIST Webbook
tf	257.55 ± 0.50	K	NIST Webbook
tf	252.05 ± 0.50	K	NIST Webbook
tf	257.55 ± 0.40	K	NIST Webbook
tf	258.50 ± 0.30	K	NIST Webbook
tf	258.37	K	KDB
tf	258.15 ± 2.00	K	NIST Webbook
tf	254.22 ± 0.15	K	NIST Webbook
tf	253.65 ± 0.20	K	NIST Webbook
tf	250.55 ± 0.60	K	NIST Webbook
tf	253.70 ± 0.50	K	NIST Webbook
tf	253.65 ± 1.00	K	NIST Webbook
tf	257.93 ± 0.05	K	NIST Webbook
tf	258.30 ± 0.30	K	NIST Webbook
tf	258.15 ± 1.00	K	NIST Webbook
tf	258.70 ± 0.20	K	NIST Webbook
tf	258.25 ± 0.30	K	NIST Webbook
tf	258.45 ± 0.30	K	NIST Webbook
tt	258.36 ± 0.00	K	NIST Webbook
vc	0.437	m3/kmol	KDB
zc	0.3266440		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	164.40	J/mol×K	290.00	NIST Webbook
cpl	194.90	J/mol×K	298.15	NIST Webbook
cpl	203.80	J/mol×K	298.00	NIST Webbook
cpl	199.20	J/mol×K	298.10	NIST Webbook
cpl	192.90	J/mol×K	302.50	NIST Webbook
cpl	192.90	J/mol×K	302.40	NIST Webbook
cpl	190.40	J/mol×K	283.00	NIST Webbook
cpl	194.89	J/mol×K	298.15	NIST Webbook
hfust	10.72	kJ/mol	257.93	NIST Webbook
hfust	0.07	kJ/mol	220.00	NIST Webbook
hfust	10.80	kJ/mol	258.40	NIST Webbook

hfust	10.66	kJ/mol	258.40	NIST Webbook
hfust	10.66	kJ/mol	258.40	NIST Webbook
hvapt	57.90 ± 0.10	kJ/mol	428.50	NIST Webbook
hvapt	46.00 ± 0.30	kJ/mol	428.50	NIST Webbook
hvapt	48.40 ± 0.20	kJ/mol	428.50	NIST Webbook
hvapt	50.70 ± 0.10	kJ/mol	428.50	NIST Webbook
hvapt	53.10 ± 0.10	kJ/mol	428.50	NIST Webbook
hvapt	55.50 ± 0.10	kJ/mol	428.50	NIST Webbook
hvapt	46.90	kJ/mol	620.50	NIST Webbook
hvapt	46.50	kJ/mol	560.00	NIST Webbook
hvapt	49.20	kJ/mol	472.00	NIST Webbook
hvapt	46.10	kJ/mol	628.50	NIST Webbook
pvap	135.00	kPa	523.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
pvap	245.00	kPa	553.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
pvap	416.00	kPa	583.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
pvap	668.00	kPa	613.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
pvap	955.00	kPa	638.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
pvap	1166.00	kPa	653.15	High-Temperature VLE for the Ethylbenzene + Quinoline System
rhol	1095.00	kg/m3	293.00	KDB

rhol	1089.30	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	1089.45	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	1089.45	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
sfust	41.79	J/mol×K	258.40	NIST Webbook
sfust	0.31	J/mol×K	220.00	NIST Webbook
sfust	41.27	J/mol×K	258.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45960e+01
Coeff. B	-4.38177e+03
Coeff. C	-7.18450e+01
Temperature range (K), min.	378.08
Temperature range (K), max.	543.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.33820e+02
Coeff. B	-1.23999e+04
Coeff. C	-1.71511e+01
Coeff. D	7.84999e-06
Temperature range (K), min.	258.25
Temperature range (K), max.	782.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Binary Liquid-Liquid Equilibrium (LLE) for N-Methylformamide (NMF) + Hexadecane between (288.15 and 313.15) K and Ternary LLE for Systems of NMF + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K:	https://www.doi.org/10.1021/je8006265
Thermochemistry of adducts of some bivalent transition metal bromides with quinoline:	https://www.doi.org/10.1016/j.tca.2007.11.018
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
(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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1362
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1362.mol
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1362
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
Vapor Pressures and Vapor-Liquid Equilibria of the 2,2,2-Trifluoroethanol + Quinoline System:	https://www.doi.org/10.1021/je025576d
High-Temperature VLE for the Ethylbenzene + Quinoline System:	https://www.doi.org/10.1021/je034107o
Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline:	https://www.doi.org/10.1016/j.jct.2008.03.015
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91225&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: Elevated Temperature and the Ternary Systems of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K:	https://www.doi.org/10.1021/acs.jced.8b00096
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
fpo:	Flash Point (Open Cup Method)
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
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
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