Quinoline, 2-methyl-

Other names:	2-METHYLCHINOLIN
	2-Methylquinoline
	Chinaldine
	KHINALDIN
	QUINALDINE
	«alpha»-Methylquinoline
	Â«alphaÂ»-Methylquinoline
Inchi:	InChI=1S/C10H9N/c1-8-6-7-9-4-2-3-5-10(9)11-8/h2-7H,1H3
InchiKey:	SMUQFGGVLNAIOZ-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1ccc2ccccc2n1
Mol. weight [g/mol]:	143.19
CAS:	91-63-4

Physical Properties

Property code	Value	Unit	Source
af	0.4060		KDB
chl	-5314.30 ± 2.10	kJ/mol	NIST Webbook
hf	159.10 ± 3.10	kJ/mol	NIST Webbook
hfl	93.00 ± 2.50	kJ/mol	NIST Webbook
hfus	12.52	kJ/mol	The thermodynamic properties of 2-methylquinoline and 8 methylquinoline
hvap	66.10 ± 1.90	kJ/mol	NIST Webbook
hvap	62.60 ± 0.10	kJ/mol	NIST Webbook
hvap	66.10 ± 1.90	kJ/mol	NIST Webbook
hvap	66.10	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4900.00	kPa	KDB
rinpol	1287.20		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	223.47		NIST Webbook
rinpol	223.94		NIST Webbook
rinpol	224.13		NIST Webbook
rinpol	223.47		NIST Webbook

rinpol	1277.50		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1287.20		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1940.00		NIST Webbook
tb	519.00 ± 6.00	K	NIST Webbook
tb	519.95 ± 0.60	K	NIST Webbook
tb	520.15 ± 2.00	K	NIST Webbook
tb	520.00 ± 10.00	K	NIST Webbook
tb	519.00 ± 5.00	K	NIST Webbook
tb	520.35 ± 0.60	K	NIST Webbook
tb	519.80 ± 0.30	K	NIST Webbook
tb	520.90 ± 0.07	K	NIST Webbook
tb	521.15 ± 0.70	K	NIST Webbook
tb	520.90 ± 0.17	K	NIST Webbook
tb	521.20	K	NIST Webbook
tb	520.90	K	KDB
tb	518.95 ± 0.40	K	NIST Webbook
tc	787.00	K	KDB
tf	271.00	K	KDB
tf	270.30 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	12.52	kJ/mol	270.50	NIST Webbook
hvapt	50.40 ± 0.10	kJ/mol	436.00	NIST Webbook

hvapt	61.00 ± 0.10	kJ/mol	436.00	NIST Webbook
hvapt	58.20 ± 0.10	kJ/mol	436.00	NIST Webbook
hvapt	55.60 ± 0.10	kJ/mol	436.00	NIST Webbook
hvapt	53.00 ± 0.10	kJ/mol	436.00	NIST Webbook
hvapt	47.70 ± 0.20	kJ/mol	436.00	NIST Webbook
hvapt	54.70	kJ/mol	482.00	NIST Webbook
hvapt	61.20	kJ/mol	297.00	NIST Webbook
rhol	1059.59	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45182e+01
Coeff. B	-4.43929e+03
Coeff. C	-7.15800e+01
Temperature range (K), min.	383.53
Temperature range (K), max.	553.76

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The thermodynamic properties of 2-methylquinoline and 8 methylquinoline:	https://www.doi.org/10.1021/je049595u
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1365.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91634&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions

hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point