Quinoline, 7-methyl-

Other names:	7-Methylquinoline
	M-TOLUQUINOLINE
Inchi:	InChI=1S/C10H9N/c1-8-4-5-9-3-2-6-11-10(9)7-8/h2-7H,1H3
InchiKey:	KDYVCOSVYOSHOL-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1ccc2cccnc2c1
Mol. weight [g/mol]:	143.19
CAS:	612-60-2

Physical Properties

Property code	Value	Unit	Source
af	0.3860		KDB
log10ws	-3.52		Crippen Method
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	3700.00	kPa	KDB
rinpol	1354.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	230.99		NIST Webbook
rinpol	231.46		NIST Webbook
rinpol	231.37		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1338.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	525.15 ± 2.00	K	NIST Webbook

tb	525.15 ± 0.70	K	NIST Webbook
tb	530.86 ± 0.18	K	NIST Webbook
tb	530.80	K	NIST Webbook
tb	583.30	K	KDB
tb	529.00 ± 2.00	K	NIST Webbook
tc	797.00	K	KDB
tf	306.00	K	KDB
tf	312.70 ± 0.20	K	NIST Webbook
tf	311.00 ± 2.00	K	NIST Webbook
tf	311.00 ± 2.00	K	NIST Webbook
tf	310.70 ± 0.50	K	NIST Webbook
tf	311.30 ± 0.40	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.70	kJ/mol	512.50	NIST Webbook
rhol	1059.59	kg/m3	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40019e+01
Coeff. B	-4.14817e+03
Coeff. C	-8.87350e+01
Temperature range (K), min.	391.20
Temperature range (K), max.	566.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.57517e+01
Coeff. B	-9.48390e+03
Coeff. C	-7.00232e+00
Coeff. D	2.37010e-06
Temperature range (K), min.	511.15
Temperature range (K), max.	531.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1369.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C612602&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1369

Legend

af:	Acentric Factor
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point