Quinoline, 6-methyl-

Other names:	6-Methylquinoline
	P-METHYLQUINOLINE
	P-TOLUQUINOLINE
Inchi:	InChI=1S/C10H9N/c1-8-4-5-10-9(7-8)3-2-6-11-10/h2-7H,1H3
InchiKey:	LUYISICIYVKBTA-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1ccc2ncccc2c1
Mol. weight [g/mol]:	143.19
CAS:	91-62-3

Physical Properties

Property code	Value	Unit	Source
chl	-5314.60 ± 2.00	kJ/mol	NIST Webbook
hf	161.00 ± 3.00	kJ/mol	NIST Webbook
hfl	93.30	kJ/mol	NIST Webbook
hvap	67.70	kJ/mol	NIST Webbook
hvap	67.70 ± 1.80	kJ/mol	NIST Webbook
hvap	67.70 ± 1.80	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
rinpol	1321.20		NIST Webbook
rinpol	1321.20		NIST Webbook
rinpol	230.75		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	230.75		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	229.82		NIST Webbook
rinpol	1343.00		NIST Webbook
ripol	2016.00		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
ripol	2020.00		NIST Webbook
ripol	2062.00		NIST Webbook
tb	538.18 ± 0.05	K	NIST Webbook
tb	531.80	K	NIST Webbook
tb	530.15 ± 0.70	K	NIST Webbook
tb	525.65 ± 3.00	K	NIST Webbook
tb	532.15 ± 1.00	K	NIST Webbook
tb	532.40 ± 0.30	K	NIST Webbook
tb	527.00 ± 2.00	K	NIST Webbook
tb	538.20 ± 0.20	K	NIST Webbook
tf	305.60 ± 0.40	K	NIST Webbook
tf	305.60 ± 0.20	K	NIST Webbook
tf	247.15 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.10	kJ/mol	496.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44514e+01
Coeff. B	-4.33852e+03
Coeff. C	-9.07810e+01
Temperature range (K), min.	397.09
Temperature range (K), max.	565.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.36389e+02

Coeff. B	-1.34466e+04
Coeff. C	-1.72949e+01
Coeff. D	6.79359e-06
Temperature range (K), min.	459.15
Temperature range (K), max.	539.15

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/mol1368.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91623&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=1368

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point