

Quinoline, 4-methyl-

Other names:	4-Lepidine 4-Methylquinoline Cincholepidine LEPIDIN LEPIDINE P-METHYLQUINOLINE «gamma»-Methylquinoline Â«gammaÂ»-Methylquinoline
Inchi:	InChI=1S/C10H9N/c1-8-6-7-11-10-5-3-2-4-9(8)10/h2-7H,1H3
InchiKey:	MUDSDYNRBDKLGK-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1ccnc2ccccc12
Mol. weight [g/mol]:	143.19
CAS:	491-35-0

Physical Properties

Property code	Value	Unit	Source
af	0.4810		KDB
chl	-5315.90 ± 2.40	kJ/mol	NIST Webbook
hf	162.10 ± 3.20	kJ/mol	NIST Webbook
hfl	94.50 ± 2.60	kJ/mol	NIST Webbook
hvap	67.60 ± 1.80	kJ/mol	NIST Webbook
hvap	67.60	kJ/mol	NIST Webbook
hvap	67.60 ± 1.80	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	1383.00		NIST Webbook
rinpol	236.61		NIST Webbook
rinpol	235.77		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	235.54		NIST Webbook

ripol	1399.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	235.54		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2066.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2098.00		NIST Webbook
tb	534.00 ± 5.00	K	NIST Webbook
tb	538.80 ± 0.30	K	NIST Webbook
tb	534.00 ± 5.00	K	NIST Webbook
tb	530.15 ± 0.70	K	NIST Webbook
tb	538.80 ± 0.20	K	NIST Webbook
tb	535.20	K	NIST Webbook
tb	538.80	K	KDB
tb	534.00 ± 6.00	K	NIST Webbook
tc	797.00	K	KDB
tf	282.00 ± 1.50	K	NIST Webbook
tf	282.70 ± 0.20	K	NIST Webbook
tf	282.00	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	58.20	kJ/mol	501.00	NIST Webbook
rhol	1088.23	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49235e+01
Coeff. B	-4.51779e+03
Coeff. C	-9.65980e+01
Temperature range (K), min.	405.28
Temperature range (K), max.	566.61

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C491350&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1367.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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