Quinoline, 1,2,3,4-tetrahydro-

Other names:	Kusol
	1,2,3,4-Tetrahydroquinoline
	Tetrahydroquinoline
	1,2,3,4-Tetrahydrochinoline
Inchi:	InChI=1S/C9H11N/c1-2-6-9-8(4-1)5-3-7-10-9/h1-2,4,6,10H,3,5,7H2
InchiKey:	LBUJPTNKIBCYBY-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	c1ccc2c(c1)CCCN2
Mol. weight [g/mol]:	133.19
CAS:	635-46-1

Physical Properties

Property code	Value	Unit	Source
chl	-5130.34 ± 0.66	kJ/mol	NIST Webbook
gf	271.75	kJ/mol	Joback Method
hf	82.00 ± 0.80	kJ/mol	NIST Webbook
hfl	16.70 ± 0.80	kJ/mol	NIST Webbook
hfus	17.27	kJ/mol	Joback Method
hvap	65.30 ± 0.20	kJ/mol	NIST Webbook
hvap	65.30	kJ/mol	NIST Webbook
hvap	65.33	kJ/mol	NIST Webbook
ie	7.61	eV	NIST Webbook
ie	7.00 ± 0.02	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.045		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
rinpol	1326.80		NIST Webbook
rinpol	225.97		NIST Webbook
rinpol	225.97		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1325.10		NIST Webbook
rinpol	1318.50		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1332.50		NIST Webbook
rinpol	1285.00		NIST Webbook

rinpol	1294.90		NIST Webbook
rinpol	1318.50		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1332.50		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1325.10		NIST Webbook
sl	240.36	J/mol×K	NIST Webbook
tb	524.00 ± 1.00	K	NIST Webbook
tb	522.20	K	NIST Webbook
tc	743.80	K	Joback Method
tf	353.82	K	Joback Method
tt	289.91 ± 0.01	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.58	J/mol×K	743.80	Joback Method
cpg	254.56	J/mol×K	541.64	Joback Method
cpg	268.91	J/mol×K	582.07	Joback Method
cpg	282.22	J/mol×K	622.51	Joback Method
cpg	294.57	J/mol×K	662.94	Joback Method
cpg	306.00	J/mol×K	703.37	Joback Method
cpg	239.11	J/mol×K	501.21	Joback Method
cpl	236.04	J/mol×K	298.15	NIST Webbook
hfust	11.81	kJ/mol	290.00	NIST Webbook
hfust	11.81	kJ/mol	290.00	NIST Webbook
hvapt	62.10 ± 0.10	kJ/mol	447.50	NIST Webbook
hvapt	59.20 ± 0.10	kJ/mol	447.50	NIST Webbook
hvapt	56.30 ± 0.10	kJ/mol	447.50	NIST Webbook
hvapt	53.50 ± 0.20	kJ/mol	447.50	NIST Webbook
hvapt	50.80 ± 0.30	kJ/mol	447.50	NIST Webbook
hvapt	47.90 ± 0.40	kJ/mol	447.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C635461&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume