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

Other names:	1,2,3,4-Tetrahydrochinoline
	1,2,3,4-Tetrahydroquinoline
	Kusol
	Tetrahydroquinoline
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
af	0.4025		Cheméo Relay (1.0)
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
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	-1.76		Cheméo Relay (1.0)
logp	2.045		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
rinpol	1332.50		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1318.50		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
rinpol	225.97		NIST Webbook
rinpol	1326.80		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	225.97		NIST Webbook
rinpol	1325.10		NIST Webbook
rinpol	1326.80		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	784.52	K	Cheméo Relay (1.0)
tf	290.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
tt	289.91 ± 0.01	K	NIST Webbook
tt	289.91 ± 0.01	K	NIST Webbook
vc	0.401	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	50.80 ± 0.30	kJ/mol	447.50	NIST Webbook
hvapt	47.90 ± 0.40	kJ/mol	447.50	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
hvapt	53.50 ± 0.20	kJ/mol	447.50	NIST Webbook
hvapt	56.30 ± 0.10	kJ/mol	447.50	NIST Webbook
hvapt	59.20 ± 0.10	kJ/mol	447.50	NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-6.92800e+01
Coeff. B	8.74800e-01
Coeff. C	-5.98560e-04
Coeff. D	1.61200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C635461&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

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https://www.chemeo.com/cid/21-194-3/Quinoline-1-2-3-4-tetrahydro.pdf
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