Isoquinoline, 1,2,3,4-tetrahydro-

Other names:	1,2,3,4-Tetrahydroisoquinoline
	Tetrahydroisoquinoline
	1,2,3,4-Tetrahydro-2-isoquinoline
	1,2,3,4-Tetrahydro-2-azanaphthalene
Inchi:	InChI=1S/C9H11N/c1-2-4-9-7-10-6-5-8(9)3-1/h1-4,10H,5-7H2
InchiKey:	UWYZHKAOTLEWKK-UHFFFAOYSA-N
Formula:	C9H11N
SMILES:	c1ccc2c(c1)CCNC2
Mol. weight [g/mol]:	133.19
CAS:	91-21-4

Physical Properties

Property code	Value	Unit	Source
gf	271.75	kJ/mol	Joback Method
hf	120.76	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
ie	8.63	eV	NIST Webbook
ie	8.57 ± 0.05	eV	NIST Webbook
log10ws	-2.24		Crippen Method
logp	1.332		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
tb	505.70	K	NIST Webbook
tc	743.80	K	Joback Method
tf	353.82	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.11	J/mol×K	501.21	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	316.58	J/mol×K	743.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91214&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume