1H-Indole, 2,3-dihydro-

Other names:	1-Azaindan
	2,3-Dihydro-1H-Indole
	2,3-Dihydroindole
	Dihydroindole
	Indole, 2,3-dihydro-
	Indolene
	Indoline
Inchi:	InChI=1S/C8H9N/c1-2-4-8-7(3-1)5-6-9-8/h1-4,9H,5-6H2
InchiKey:	LPAGFVYQRIESJQ-UHFFFAOYSA-N
Formula:	C8H9N
SMILES:	c1ccc2c(c1)CCN2
Mol. weight [g/mol]:	119.16
CAS:	496-15-1

Physical Properties

Property code	Value	Unit	Source
affp	957.10	kJ/mol	NIST Webbook
basg	926.30	kJ/mol	NIST Webbook
gf	275.43	kJ/mol	Joback Method
hf	147.56	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	61.90 ± 1.70	kJ/mol	NIST Webbook
ie	7.15 ± 0.02	eV	NIST Webbook
log10ws	-1.04		Estimated Solubility Method
log10ws	-1.04		Aqueous Solubility Prediction Method
logp	1.655		Crippen Method
mcvol	98.940	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
rinpol	1195.80		NIST Webbook
rinpol	1195.80		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	204.74		NIST Webbook
rinpol	204.74		NIST Webbook
tb	503.00 ± 4.00	K	NIST Webbook
tb	493.70	K	NIST Webbook

tb	502.20	K	NIST Webbook
tc	711.60	K	Joback Method
tf	346.07	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.35	J/mol×K	474.06	Joback Method
cpg	210.70	J/mol×K	513.65	Joback Method
cpg	223.07	J/mol×K	553.24	Joback Method
cpg	234.52	J/mol×K	592.83	Joback Method
cpg	245.11	J/mol×K	632.42	Joback Method
cpg	254.92	J/mol×K	672.01	Joback Method
cpg	264.02	J/mol×K	711.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.70	K	0.30	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C496151&Units=SI

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

Extraction of nitrogen compounds from diesel fuel using imidazolium- and pyridinium- based ionic liquids: Experiments, COSMO-RS prediction and NRTL correlation: https://www.doi.org/10.1016/j.fluid.2015.07.021

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume