Indane

Other names:	1,2-Hydrindene
	1H-Indene, 2,3-dihydro-
	2,3-DIHYDROINDENE
	2,3-Dihydro-1H-indene
	Benzocyclopentane
	Hydrindene
	Hydrindonaphthene
	INDAN
	Indene, 2,3-dihydro-
	NSC 5292
Inchi:	InChI=1S/C9H10/c1-2-5-9-7-3-6-8(9)4-1/h1-2,4-5H,3,6-7H2
InchiKey:	PQNFLJBBNBOBRQ-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	c1ccc2c(c1)CCC2
Mol. weight [g/mol]:	118.18
CAS:	496-11-7

Physical Properties

Property code	Value	Unit	Source
af	0.3080		KDB
chl	-4982.50 ± 1.40	kJ/mol	NIST Webbook
chl	-4981.60 ± 2.00	kJ/mol	NIST Webbook
gf	196.14	kJ/mol	Joback Method
hf	60.70 ± 1.50	kJ/mol	NIST Webbook
hf	59.70 ± 2.00	kJ/mol	NIST Webbook
hf	60.90 ± 2.10	kJ/mol	NIST Webbook
hfl	11.70 ± 1.80	kJ/mol	NIST Webbook
hfl	10.70 ± 2.00	kJ/mol	NIST Webbook
hfl	11.70 ± 1.50	kJ/mol	NIST Webbook
hfus	9.78	kJ/mol	Joback Method
hvap	48.80	kJ/mol	NIST Webbook
hvap	49.03 ± 0.20	kJ/mol	NIST Webbook
hvap	49.20 ± 1.00	kJ/mol	NIST Webbook
hvap	49.00	kJ/mol	NIST Webbook
ie	8.60 ± 0.01	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.46 ± 0.03	eV	NIST Webbook

ie	8.45 ± 0.02	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
ie	9.05 ± 0.05	eV	NIST Webbook
log10ws	-3.03		Aqueous Solubility Prediction Method
log10ws	-3.04		Estimated Solubility Method
logp	2.175		Crippen Method
mcvol	103.050	ml/mol	McGowan Method
pc	3950.00 ± 40.00	kPa	NIST Webbook
pc	3950.00 ± 30.00	kPa	NIST Webbook
pc	3950.00	kPa	KDB
rinpol	1035.50		NIST Webbook
rinpol	1015.70		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1011.20		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1027.40		NIST Webbook
rinpol	1036.10		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1011.20		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1011.20		NIST Webbook
rinpol	1014.50		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1011.80		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1019.45		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1024.50		NIST Webbook

rinpol	1027.40	NIST Webbook
rinpol	1032.40	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1047.80	NIST Webbook
rinpol	1017.40	NIST Webbook
rinpol	1027.40	NIST Webbook
rinpol	1032.40	NIST Webbook
rinpol	1035.50	NIST Webbook
rinpol	1015.41	NIST Webbook
rinpol	1015.61	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1007.28	NIST Webbook
rinpol	1058.00	NIST Webbook
rinpol	1016.71	NIST Webbook
rinpol	1030.81	NIST Webbook
rinpol	1036.70	NIST Webbook
rinpol	1041.08	NIST Webbook
rinpol	1013.00	NIST Webbook
rinpol	1039.25	NIST Webbook
rinpol	1038.00	NIST Webbook
rinpol	1046.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1036.00	NIST Webbook
rinpol	1019.00	NIST Webbook
rinpol	1032.00	NIST Webbook
rinpol	1026.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1020.00	NIST Webbook
rinpol	1023.00	NIST Webbook
rinpol	1027.00	NIST Webbook
rinpol	1002.00	NIST Webbook
rinpol	1033.00	NIST Webbook
rinpol	1017.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1029.00	NIST Webbook
rinpol	1034.00	NIST Webbook
rinpol	1041.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1013.00	NIST Webbook

rinpol	1013.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	169.10		NIST Webbook
rinpol	168.83		NIST Webbook
rinpol	170.21		NIST Webbook
rinpol	168.87		NIST Webbook
rinpol	165.50		NIST Webbook
rinpol	167.82		NIST Webbook
rinpol	168.87		NIST Webbook
rinpol	169.87		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	1066.70		NIST Webbook
rinpol	1050.80		NIST Webbook
rinpol	169.04		NIST Webbook
rinpol	1013.03		NIST Webbook
rinpol	1014.50		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1355.90		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1355.90		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1365.00		NIST Webbook
sl	234.35	J/mol×K	NIST Webbook
sl	234.34	J/mol×K	NIST Webbook
tb	451.12	K	KDB
tc	684.90	K	KDB
tc	684.90 ± 0.50	K	NIST Webbook
tc	684.90 ± 0.40	K	NIST Webbook
tc	684.90	K	NIST Webbook
tf	221.70	K	KDB
tf	221.95	K	Aqueous Solubility Prediction Method
tf	221.46 ± 0.40	K	NIST Webbook
tt	221.77 ± 0.02	K	NIST Webbook

tt	221.79	K	Thermodynamic properties of indan: Experimental and computational results
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.64 ± 0.39	J/mol×K	435.65	NIST Webbook
cpg	199.15 ± 0.39	J/mol×K	448.15	NIST Webbook
cpg	209.22 ± 0.39	J/mol×K	473.15	NIST Webbook
cpg	219.20 ± 0.39	J/mol×K	498.15	NIST Webbook
cpg	228.37 ± 0.39	J/mol×K	523.15	NIST Webbook
cpl	190.25	J/mol×K	298.15	NIST Webbook
cpl	190.25	J/mol×K	298.15	NIST Webbook
dvisc	0.0005359	Pa×s	383.03	Joback Method
dvisc	0.0004481	Pa×s	415.71	Joback Method
dvisc	0.0006627	Pa×s	350.35	Joback Method
dvisc	0.0003846	Pa×s	448.39	Joback Method
dvisc	0.0017430	Pa×s	252.31	Joback Method
dvisc	0.0011727	Pa×s	284.99	Joback Method
dvisc	0.0008561	Pa×s	317.67	Joback Method
hfust	8.60	kJ/mol	221.77	NIST Webbook
hfust	8.60	kJ/mol	221.80	NIST Webbook
hfust	8.60	kJ/mol	221.80	NIST Webbook
hvapt	45.00	kJ/mol	418.50	NIST Webbook
hvapt	44.00	kJ/mol	420.00	NIST Webbook
hvapt	39.63	kJ/mol	451.00	NIST Webbook
rfi	1.53580		298.15	KDB
sfust	38.77	J/mol×K	221.77	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67689e+01
Coeff. B	-4.58687e+03
Coeff. C	-5.13930e+01

Temperature range (K), min.	329.70
Temperature range (K), max.	451.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.37734e+01
Coeff. B	-8.59035e+03
Coeff. C	-1.00029e+01
Coeff. D	5.02936e-06
Temperature range (K), min.	221.74
Temperature range (K), max.	684.90

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C496117&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol751.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=751
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of indan:	https://www.doi.org/10.1016/j.jct.2015.12.005
Experimental and computational results:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
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