1H-Indene, octahydro-, cis-

Other names:	Indan, hexahydro-, cis- Indene, octahydro-, cis- Octahydro-1H-indene, cis cis-Bicyclo[4.3.0]Nonane cis-Hexahydroindan cis-Hydrindan cis-Hydrindane cis-Octahydro-1H-indene cis-Perhydroindene cis-hexahydrindan
Inchi:	InChI=1S/C9H16/c1-2-5-9-7-3-6-8(9)4-1/h8-9H,1-7H2/t8-,9+
InchiKey:	BNRNAKTVFSZAFA-DTORHVGOSA-N
Formula:	C9H16
SMILES:	C1CCC2CCCC2C1
Mol. weight [g/mol]:	124.22
CAS:	4551-51-3

Physical Properties

Property code	Value	Unit	Source
chl	-5655.10 ± 1.50	kJ/mol	NIST Webbook
chl	-5646.70 ± 5.90	kJ/mol	NIST Webbook
gf	110.10	kJ/mol	Joback Method
hf	-127.20 ± 2.00	kJ/mol	NIST Webbook
hfl	-173.30 ± 1.50	kJ/mol	NIST Webbook
hfus	9.04	kJ/mol	Joback Method
hvap	46.10	kJ/mol	NIST Webbook
hvap	46.00 ± 1.30	kJ/mol	NIST Webbook
ie	9.50 ± 0.00	eV	NIST Webbook
ie	9.46 ± 0.06	eV	NIST Webbook
ie	10.13 ± 0.03	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	2.977		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	981.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	984.00		NIST Webbook

rinpol	975.00		NIST Webbook
rinpol	1035.60		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1035.60		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	1033.10		NIST Webbook
rinpol	1012.70		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	980.90		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	985.80		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	985.80		NIST Webbook
rinpol	989.50		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	989.50		NIST Webbook
rinpol	996.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1107.30		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1156.00		NIST Webbook
sl	265.47	J/mol×K	NIST Webbook
tb	441.01 ± 0.20	K	NIST Webbook
tb	441.07 ± 0.50	K	NIST Webbook

tb	441.07 ± 0.20	K	NIST Webbook
tb	440.97 ± 0.50	K	NIST Webbook
tb	441.01 ± 0.25	K	NIST Webbook
tb	440.89 ± 0.30	K	NIST Webbook
tb	440.93 ± 0.30	K	NIST Webbook
tb	440.93 ± 0.40	K	NIST Webbook
tb	437.00 ± 3.00	K	NIST Webbook
tc	647.88	K	Joback Method
tf	216.51	K	Joback Method
tt	236.48 ± 0.01	K	NIST Webbook
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.94	J/mol×K	431.61	Joback Method
cpg	261.35	J/mol×K	467.66	Joback Method
cpg	280.52	J/mol×K	503.70	Joback Method
cpg	298.50	J/mol×K	539.75	Joback Method
cpg	315.35	J/mol×K	575.79	Joback Method
cpg	331.12	J/mol×K	611.84	Joback Method
cpg	345.88	J/mol×K	647.88	Joback Method
cpl	214.18	J/mol×K	298.15	NIST Webbook
dvisc	0.0026731	Pa×s	216.51	Joback Method
dvisc	0.0016168	Pa×s	252.36	Joback Method
dvisc	0.0011082	Pa×s	288.21	Joback Method
dvisc	0.0008258	Pa×s	324.06	Joback Method
dvisc	0.0006525	Pa×s	359.91	Joback Method
dvisc	0.0004581	Pa×s	431.61	Joback Method
dvisc	0.0005380	Pa×s	395.76	Joback Method
hfust	1.40	kJ/mol	236.50	NIST Webbook
hfust	8.26	kJ/mol	182.30	NIST Webbook
hfust	0.39	kJ/mol	184.50	NIST Webbook
hfust	1.40	kJ/mol	236.50	NIST Webbook
hvapt	47.10	kJ/mol	278.00	NIST Webbook
hvapt	45.90	kJ/mol	328.00	NIST Webbook
hvapt	41.90	kJ/mol	413.00	NIST Webbook
hvapt	42.60	kJ/mol	396.00	NIST Webbook
sfust	45.33	J/mol×K	182.30	NIST Webbook
sfust	2.13	J/mol×K	184.50	NIST Webbook
sfust	5.91	J/mol×K	236.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39968e+01
Coeff. B	-3.49920e+03
Coeff. C	-6.61020e+01
Temperature range (K), min.	321.35
Temperature range (K), max.	468.99

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4551513&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
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