1H-Indene, octahydro-, trans-

Other names:	Indene, octahydro-, trans- Octahydro-1H-indene, trans indan, hexahydro-, trans- trans-Hexahydrindan trans-bicyclo[4.3.0]nonane trans-hexahydroindan trans-hydrindan trans-hydrindane trans-octahydro-1H-indene trans-perhydroindene
Inchi:	InChI=1S/C9H16/c1-2-5-9-7-3-6-8(9)4-1/h8-9H,1-7H2/t8-,9-/m0/s1
InchiKey:	BNRNAKTVFSZAFA-IUCAKERBSA-N
Formula:	C9H16
SMILES:	C1CCC2CCCC2C1
Mol. weight [g/mol]:	124.22
CAS:	3296-50-2

Physical Properties

Property code	Value	Unit	Source
chl	-5652.00 ± 1.70	kJ/mol	NIST Webbook
chl	-5640.90 ± 5.90	kJ/mol	NIST Webbook
gf	110.10	kJ/mol	Joback Method
hf	-131.60 ± 2.10	kJ/mol	NIST Webbook
hfl	-176.40 ± 1.70	kJ/mol	NIST Webbook
hfus	9.04	kJ/mol	Joback Method
hvap	44.80 ± 1.30	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
ie	9.46 ± 0.06	eV	NIST Webbook
ie	10.18 ± 0.03	eV	NIST Webbook
ie	9.55 ± 0.00	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	947.70		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	955.00		NIST Webbook

rinpol	964.00		NIST Webbook
rinpol	955.30		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	947.70		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	955.30		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	949.80		NIST Webbook
rinpol	999.80		NIST Webbook
rinpol	1001.90		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1059.30		NIST Webbook
ripol	1059.00		NIST Webbook
sl	258.86	J/mol×K	NIST Webbook
tb	434.21 ± 0.15	K	NIST Webbook
tb	434.21 ± 0.30	K	NIST Webbook
tb	434.24 ± 0.30	K	NIST Webbook
tb	434.21 ± 0.20	K	NIST Webbook
tb	434.24 ± 0.20	K	NIST Webbook
tb	434.17 ± 0.10	K	NIST Webbook
tb	434.23 ± 0.02	K	NIST Webbook
tb	434.21 ± 0.20	K	NIST Webbook
tb	434.21 ± 0.20	K	NIST Webbook
tc	647.88	K	Joback Method
tf	216.51	K	Joback Method
tt	213.80 ± 0.20	K	NIST Webbook
tt	213.86 ± 0.01	K	NIST Webbook
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.88	J/mol×K	647.88	Joback Method
cpg	331.12	J/mol×K	611.84	Joback Method
cpg	315.35	J/mol×K	575.79	Joback Method
cpg	298.50	J/mol×K	539.75	Joback Method
cpg	280.52	J/mol×K	503.70	Joback Method

cpg	261.35	J/mol×K	467.66	Joback Method
cpg	240.94	J/mol×K	431.61	Joback Method
cpl	209.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0006525	Pa×s	359.91	Joback Method
dvisc	0.0026731	Pa×s	216.51	Joback Method
dvisc	0.0004581	Pa×s	431.61	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	0.0005380	Pa×s	395.76	Joback Method
hfust	10.90	kJ/mol	213.90	NIST Webbook
hfust	10.91	kJ/mol	213.86	NIST Webbook
hvapt	41.10	kJ/mol	406.50	NIST Webbook
hvapt	41.60	kJ/mol	390.00	NIST Webbook
hvapt	41.00	kJ/mol	418.50	NIST Webbook
hvapt	45.90	kJ/mol	272.50	NIST Webbook
hvapt	45.10	kJ/mol	321.50	NIST Webbook
sfust	50.99	J/mol×K	213.86	NIST Webbook

Sources

Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3296502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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