1H-Indene, 3a,4,7,7a-tetrahydro-

Other names:	3a,4,7,7a-Tetrahydro-1H-indene
	3a,4,7,7a-Tetrahydroindene
	4,7,8,9-Tetrahydroindene
	Bicyclo(4,3,0)nona-3,7-diene
	Bicyclo[4.3.0]nona-3,7-diene
	Indene, 3a,4,7,7a-tetrahydro-
	Tetrahydroindene
Inchi:	InChI=1S/C9H12/c1-2-5-9-7-3-6-8(9)4-1/h1-3,6,8-9H,4-5,7H2
InchiKey:	UFERIGCCDYCZLN-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C1=CCC2CC=CC2C1
Mol. weight [g/mol]:	120.19
CAS:	3048-65-5

Physical Properties

Property code	Value	Unit	Source
gf	170.02	kJ/mol	Joback Method
hf	13.59	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	36.55	kJ/mol	Joback Method
ie	8.78	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	2.529		Crippen Method
mcvol	107.350	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
tb	429.93	K	Joback Method
tc	650.87	K	Joback Method
tf	218.03	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.82	J/mol×K	650.87	Joback Method
cpg	212.74	J/mol×K	429.93	Joback Method
cpg	230.54	J/mol×K	466.75	Joback Method
cpg	247.14	J/mol×K	503.58	Joback Method
cpg	262.61	J/mol×K	540.40	Joback Method
cpg	277.00	J/mol×K	577.22	Joback Method
cpg	290.38	J/mol×K	614.05	Joback Method
dvisc	0.0004197	Pa×s	429.93	Joback Method
dvisc	0.0015390	Pa×s	218.03	Joback Method
dvisc	0.0010657	Pa×s	253.35	Joback Method
dvisc	0.0008074	Pa×s	288.66	Joback Method
dvisc	0.0006499	Pa×s	323.98	Joback Method
dvisc	0.0005459	Pa×s	359.30	Joback Method
dvisc	0.0004731	Pa×s	394.61	Joback Method
hvapt	42.30	kJ/mol	389.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58796e+01
Coeff. B	-4.71010e+03
Coeff. C	-1.41180e+01
Temperature range (K), min.	316.20
Temperature range (K), max.	459.81

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3048655&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume