1H-Indene, 2,3-dihydro-1,1,4,6-tetramethyl-

Other names:	2,3-Dihydro-1,1,4,6-tetramethyl-1H-indene
	Indan, 1,1,4,6-tetramethyl-
Inchi:	InChI=1S/C13H18/c1-9-7-10(2)11-5-6-13(3,4)12(11)8-9/h7-8H,5-6H2,1-4H3
InchiKey:	PJPNYZCIGFQVQG-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	Cc1cc(C)c2c(c1)C(C)(C)CC2
Mol. weight [g/mol]:	174.28
CAS:	941-60-6

Physical Properties

Property code	Value	Unit	Source
chl	-7556.30 ± 2.70	kJ/mol	NIST Webbook
gf	197.36	kJ/mol	Joback Method
hf	-70.40 ± 2.80	kJ/mol	NIST Webbook
hfl	-131.80 ± 2.80	kJ/mol	NIST Webbook
hfus	14.14	kJ/mol	Joback Method
hvap	61.40 ± 0.50	kJ/mol	NIST Webbook
hvap	61.37 ± 0.47	kJ/mol	NIST Webbook
log10ws	-4.02		Crippen Method
logp	3.527		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1350.00		NIST Webbook
sl	348.00	J/mol×K	NIST Webbook
tb	545.44	K	Joback Method
tc	769.28	K	Joback Method
tf	342.09	K	Joback Method
tt	273.51 ± 0.02	K	NIST Webbook
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	379.74	J/mol×K	545.44	Joback Method
cpg	397.09	J/mol×K	582.75	Joback Method
cpg	413.31	J/mol×K	620.05	Joback Method
cpg	428.55	J/mol×K	657.36	Joback Method
cpg	442.97	J/mol×K	694.67	Joback Method
cpg	456.71	J/mol×K	731.97	Joback Method
cpg	469.93	J/mol×K	769.28	Joback Method
cpl	299.60	J/mol×K	298.15	NIST Webbook
hfust	15.74	kJ/mol	273.60	NIST Webbook
hvapt	59.40	kJ/mol	348.00	NIST Webbook
hvapt	60.20	kJ/mol	391.00	NIST Webbook
hvapt	51.90	kJ/mol	446.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33185e+01
Coeff. B	-3.92519e+03
Coeff. C	-8.72710e+01
Temperature range (K), min.	388.49
Temperature range (K), max.	577.49

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=C941606&Units=SI

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

Legend

chl: Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
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
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
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