1H-Indene, 2,3-dihydro-1,1-dimethyl-

Other names:	1,1-Dimethyl-(2,3-dihydroindene)
	1,1-Dimethyl-2,3-dihydro-1H-indene
	1,1-Dimethylindan
	1,1-Dimethylindane
	Indan, 1,1-dimethyl-
Inchi:	InChI=1S/C11H14/c1-11(2)8-7-9-5-3-4-6-10(9)11/h3-6H,7-8H2,1-2H3
InchiKey:	UTTMVTDJCFSOFF-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	CC1(C)CCc2ccccc21
Mol. weight [g/mol]:	146.23
CAS:	4912-92-9

Physical Properties

Property code	Value	Unit	Source
chl	-6275.62 ± 0.84	kJ/mol	NIST Webbook
chl	-6275.90 ± 1.80	kJ/mol	NIST Webbook
gf	199.78	kJ/mol	Joback Method
hf	-1.90 ± 1.00	kJ/mol	NIST Webbook
hf	-1.60 ± 1.90	kJ/mol	NIST Webbook
hfl	-53.80 ± 1.00	kJ/mol	NIST Webbook
hfl	-53.50 ± 1.90	kJ/mol	NIST Webbook
hfus	9.73	kJ/mol	Joback Method
hvap	51.90 ± 0.30	kJ/mol	NIST Webbook
hvap	51.94 ± 0.29	kJ/mol	NIST Webbook
ie	8.47	eV	NIST Webbook
log10ws	-3.06		Crippen Method
logp	2.910		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1081.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1095.00		NIST Webbook
sl	288.10	J/mol×K	NIST Webbook
tb	464.20	K	NIST Webbook
tc	719.26	K	Joback Method
tf	294.51	K	Joback Method
tt	227.35 ± 0.01	K	NIST Webbook

vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.80	J/mol×K	489.72	Joback Method
cpg	359.10	J/mol×K	681.00	Joback Method
cpg	346.71	J/mol×K	642.75	Joback Method
cpg	333.45	J/mol×K	604.49	Joback Method
cpg	319.17	J/mol×K	566.23	Joback Method
cpg	303.67	J/mol×K	527.98	Joback Method
cpg	370.81	J/mol×K	719.26	Joback Method
cpl	249.40	J/mol×K	298.15	NIST Webbook
hfust	11.99	kJ/mol	227.40	NIST Webbook
hfust	11.99	kJ/mol	227.40	NIST Webbook
hfust	11.99	kJ/mol	227.35	NIST Webbook
hvapt	50.50	kJ/mol	390.00	NIST Webbook
hvapt	50.10	kJ/mol	330.50	NIST Webbook
hvapt	45.90	kJ/mol	427.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30114e+01
Coeff. B	-3.34583e+03
Coeff. C	-7.53810e+01
Temperature range (K), min.	338.34
Temperature range (K), max.	509.91

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4912929&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
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
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