1H-Indene, 2,3-dihydro-4,7-dimethyl-

Other names:	2,3-Dihydro-4,7-dimethyl-1H-indene
	4,7-Dimethyl-(2,3-dihydroindene)
	4,7-Dimethylindan
	Indan, 4,7-dimethyl-
Inchi:	InChI=1S/C11H14/c1-8-6-7-9(2)11-5-3-4-10(8)11/h6-7H,3-5H2,1-2H3
InchiKey:	IWHKMCQFAMHMSX-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	Cc1ccc(C)c2c1CCC2
Mol. weight [g/mol]:	146.23
CAS:	6682-71-9

Physical Properties

Property code	Value	Unit	Source
chl	-6263.70 ± 1.50	kJ/mol	NIST Webbook
gf	193.72	kJ/mol	Joback Method
hf	-7.40 ± 1.70	kJ/mol	NIST Webbook
hfl	-65.70 ± 1.60	kJ/mol	NIST Webbook
hfus	14.18	kJ/mol	Joback Method
hvap	58.29 ± 0.44	kJ/mol	NIST Webbook
hvap	58.30 ± 0.40	kJ/mol	NIST Webbook
log10ws	-3.50		Crippen Method
logp	2.792		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	202.26		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1253.00		NIST Webbook
sl	293.20	J/mol×K	NIST Webbook
tb	504.11	K	Joback Method
tc	726.58	K	Joback Method
tf	299.89	K	Joback Method
tt	272.63 ± 0.01	K	NIST Webbook
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.45	J/mol×K	726.58	Joback Method
cpg	355.21	J/mol×K	689.50	Joback Method
cpg	343.21	J/mol×K	652.42	Joback Method
cpg	330.42	J/mol×K	615.34	Joback Method
cpg	316.75	J/mol×K	578.27	Joback Method
cpg	302.17	J/mol×K	541.19	Joback Method
cpg	286.59	J/mol×K	504.11	Joback Method
cpl	241.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0004962	Pa×s	436.04	Joback Method
dvisc	0.0005977	Pa×s	402.00	Joback Method
dvisc	0.0003689	Pa×s	504.11	Joback Method
dvisc	0.0013450	Pa×s	299.89	Joback Method
dvisc	0.0009713	Pa×s	333.93	Joback Method
dvisc	0.0007450	Pa×s	367.96	Joback Method
dvisc	0.0004233	Pa×s	470.07	Joback Method
hfust	13.52	kJ/mol	272.63	NIST Webbook
hfust	13.52	kJ/mol	272.70	NIST Webbook
hfust	13.52	kJ/mol	272.70	NIST Webbook
hvapt	50.60	kJ/mol	443.50	NIST Webbook
hvapt	56.90	kJ/mol	338.00	NIST Webbook
hvapt	54.70	kJ/mol	391.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46219e+01
Coeff. B	-4.34935e+03
Coeff. C	-6.42430e+01
Temperature range (K), min.	367.67
Temperature range (K), max.	531.39

Sources

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol765.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6682719&Units=SI

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
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