

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

Other names:	2,3-Dihydro-4,6-dimethyl-1H-indene 4,6-Dimethyl-(2,3-dihydroindene) 4,6-Dimethylindan Indan, 4,6-dimethyl-
Inchi:	InChI=1S/C11H14/c1-8-6-9(2)11-5-3-4-10(11)7-8/h6-7H,3-5H2,1-2H3
InchiKey:	BSYQUYXSAFIGLB-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	<chem>Cc1cc(C)c2c(c1)CCC2</chem>
Mol. weight [g/mol]:	146.23
CAS:	1685-82-1

Physical Properties

Property code	Value	Unit	Source
chl	-6265.70 ± 1.50	kJ/mol	NIST Webbook
gf	193.72	kJ/mol	Joback Method
hf	-5.80 ± 1.70	kJ/mol	NIST Webbook
hfl	-63.70 ± 1.60	kJ/mol	NIST Webbook
hfus	14.18	kJ/mol	Joback Method
hvap	57.90 ± 0.40	kJ/mol	NIST Webbook
hvap	57.91 ± 0.41	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	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	212.38		NIST Webbook
sl	295.40	J/molxK	NIST Webbook
tb	504.11	K	Joback Method
tc	726.58	K	Joback Method
tf	299.89	K	Joback Method
tt	256.45 ± 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/molxK	726.58	Joback Method
cpg	355.21	J/molxK	689.50	Joback Method
cpg	343.21	J/molxK	652.42	Joback Method
cpg	330.42	J/molxK	615.34	Joback Method
cpg	316.75	J/molxK	578.27	Joback Method
cpg	302.17	J/molxK	541.19	Joback Method
cpg	286.59	J/molxK	504.11	Joback Method
cpl	240.90	J/molxK	298.15	NIST Webbook
dvisc	0.0004962	Paxs	436.04	Joback Method
dvisc	0.0005977	Paxs	402.00	Joback Method
dvisc	0.0003689	Paxs	504.11	Joback Method
dvisc	0.0013450	Paxs	299.89	Joback Method
dvisc	0.0009713	Paxs	333.93	Joback Method
dvisc	0.0007450	Paxs	367.96	Joback Method
dvisc	0.0004233	Paxs	470.07	Joback Method
hfust	12.88	kJ/mol	256.45	NIST Webbook
hfust	12.88	kJ/mol	256.50	NIST Webbook
hfust	12.88	kJ/mol	256.50	NIST Webbook
hvapt	50.30	kJ/mol	441.00	NIST Webbook
hvapt	56.40	kJ/mol	338.00	NIST Webbook
hvapt	56.90	kJ/mol	390.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34744e+01
Coeff. B	-3.78355e+03
Coeff. C	-7.17950e+01
Temperature range (K), min.	358.71
Temperature range (K), max.	535.30

Sources

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=C1685821&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/ci990307I
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
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

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