

2,2-Dimethylindene, 2,3-dihydro-

Other names:	1H-Indene,2,3-dihydro-2,2-dimethyl-
Inchi:	InChI=1S/C11H14/c1-11(2)7-9-5-3-4-6-10(9)8-11/h3-6H,7-8H2,1-2H3
InchiKey:	VAMWEVQXIHGFHY-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	CC1(C)Cc2ccccc2C1
Mol. weight [g/mol]:	146.23
CAS:	20836-11-7

Physical Properties

Property code	Value	Unit	Source
gf	199.78	kJ/mol	Joback Method
hf	42.73	kJ/mol	Joback Method
hfus	9.73	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
ie	8.47	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	2.811		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	489.72	K	Joback Method
tc	719.26	K	Joback Method
tf	294.51	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.80	J/molxK	489.72	Joback Method
cpg	303.67	J/molxK	527.98	Joback Method
cpg	319.17	J/molxK	566.23	Joback Method
cpg	333.45	J/molxK	604.49	Joback Method
cpg	346.71	J/molxK	642.75	Joback Method
cpg	359.10	J/molxK	681.00	Joback Method
cpg	370.81	J/molxK	719.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20836117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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