

2,2-dimethylindane

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

Physical Properties

Property code	Value	Unit	Source
hf	2.54	kJ/mol	Cheméo Relay (1.0)
hfus	9.73	kJ/mol	Joback Method
hvap	51.96	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	NIST Webbook
logp	2.811		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
tb	479.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20836117&Units=SI>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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