

# 1,1,4,6,7-Pentamethylindan

<b>Inchi:</b>	InChI=1S/C14H20/c1-9-8-10(2)12-6-7-14(4,5)13(12)11(9)3/h8H,6-7H2,1-5H3
<b>InchiKey:</b>	DKEQNICHDTZGAN-UHFFFAOYSA-N
<b>Formula:</b>	C14H20
<b>SMILES:</b>	<chem>Cc1cc(C)c2c(c1C)C(C)(C)CC2</chem>
<b>Mol. weight [g/mol]:</b>	188.31
<b>CAS:</b>	6682-67-3

## Physical Properties

Property code	Value	Unit	Source
chs	-8192.30 ± 2.00	kJ/mol	NIST Webbook
gf	196.15	kJ/mol	Joback Method
hf	-53.60	kJ/mol	Joback Method
hfs	-175.10 ± 2.10	kJ/mol	NIST Webbook
hfus	16.34	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.836		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	573.30	K	Joback Method
tc	794.18	K	Joback Method
tf	365.88	K	Joback Method
vc	0.666	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.27	J/mol×K	573.30	Joback Method
cpg	445.90	J/mol×K	610.11	Joback Method
cpg	462.52	J/mol×K	646.93	Joback Method
cpg	478.25	J/mol×K	683.74	Joback Method
cpg	493.24	J/mol×K	720.55	Joback Method
cpg	507.65	J/mol×K	757.36	Joback Method
cpg	521.60	J/mol×K	794.18	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6682673&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6682673&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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