

# Benzene,[2-methyl-3-(2-methyl-1-propenylidene)c

<b>Inchi:</b>	InChI=1S/C14H16/c1-10(2)9-13-11(3)14(13)12-7-5-4-6-8-12/h4-8,11,14H,1-3H3/t11-,14-
<b>InchiKey:</b>	WBZZBXVCSQAKIK-FZMZJTMJSA-N
<b>Formula:</b>	C14H16
<b>SMILES:</b>	CC(C)=C=C1C(C)C1c1cccc1
<b>Mol. weight [g/mol]:</b>	184.28
<b>CAS:</b>	33530-27-7

## Physical Properties

Property code	Value	Unit	Source
gf	397.64	kJ/mol	Joback Method
hf	185.72	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
ie	7.63	eV	NIST Webbook
log10ws	-4.13		Crippen Method
logp	3.911		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	558.26	K	Joback Method
tc	790.01	K	Joback Method
tf	290.57	K	Joback Method
vc	0.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.28	J/molxK	558.26	Joback Method
cpg	412.76	J/molxK	596.89	Joback Method
cpg	430.03	J/molxK	635.51	Joback Method
cpg	446.17	J/molxK	674.14	Joback Method
cpg	461.23	J/molxK	712.76	Joback Method
cpg	475.28	J/molxK	751.39	Joback Method
cpg	488.39	J/molxK	790.01	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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=C33530277&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33530277&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>

# Legend

<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>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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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