

# 2,6,6-Trimethyl-1,3-cyclohexadiene

<b>Inchi:</b>	InChI=1S/C9H14/c1-8-5-4-6-9(2,3)7-8/h4-5,7H,6H2,1-3H3
<b>InchiKey:</b>	HIPJINRMIDCBDO-UHFFFAOYSA-N
<b>Formula:</b>	C9H14
<b>SMILES:</b>	CC1=CC(C)(C)CC=C1
<b>Mol. weight [g/mol]:</b>	122.21

## Physical Properties

Property code	Value	Unit	Source
gf	94.15	kJ/mol	Joback Method
hf	-55.44	kJ/mol	Joback Method
hfus	6.66	kJ/mol	Joback Method
hvap	36.15	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
ripol	962.00		NIST Webbook
tb	428.41	K	Joback Method
tc	642.33	K	Joback Method
tf	236.51	K	Joback Method
vc	0.443	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.10	J/mol×K	428.41	Joback Method
cpg	246.21	J/mol×K	464.06	Joback Method
cpg	261.18	J/mol×K	499.72	Joback Method
cpg	275.12	J/mol×K	535.37	Joback Method
cpg	288.13	J/mol×K	571.03	Joback Method
cpg	300.31	J/mol×K	606.68	Joback Method
cpg	311.78	J/mol×K	642.33	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=R547634&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R547634&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>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>ripol:</b>	Polar retention indices
<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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