

# 3,4-Octadiene, 2,2,7,7-tetramethyl-

<b>Other names:</b>	2,2,7,7-Tetramethyl-3,4-octadiene
<b>Inchi:</b>	InChI=1S/C12H22/c1-11(2,3)9-7-8-10-12(4,5)6/h7,10H,9H2,1-6H3
<b>InchiKey:</b>	APIDJYHKQJDGMH-UHFFFAOYSA-N
<b>Formula:</b>	C12H22
<b>SMILES:</b>	CC(C)(C)C=C=CCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	166.30
<b>CAS:</b>	61092-76-0

## Physical Properties

Property code	Value	Unit	Source
gf	264.34	kJ/mol	Joback Method
hf	-28.51	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.180		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
tb	474.93	K	Joback Method
tc	675.48	K	Joback Method
tf	231.27	K	Joback Method
vc	0.645	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.56	J/mol×K	474.93	Joback Method
cpg	401.55	J/mol×K	508.35	Joback Method
cpg	419.41	J/mol×K	541.78	Joback Method
cpg	436.20	J/mol×K	575.20	Joback Method
cpg	451.99	J/mol×K	608.63	Joback Method
cpg	466.82	J/mol×K	642.05	Joback Method
cpg	480.77	J/mol×K	675.48	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>
<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=C61092760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61092760&amp;Units=SI</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>h vap:</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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