

# 2,6-Dimethyl-1,6-heptadiene

<b>Inchi:</b>	InChI=1S/C9H16/c1-8(2)6-5-7-9(3)4/h1,3,5-7H2,2,4H3
<b>InchiKey:</b>	JYTKDPUEUXPAOI-UHFFFAOYSA-N
<b>Formula:</b>	C9H16
<b>SMILES:</b>	<chem>C=C(C)CCCC(=C)C</chem>
<b>Mol. weight [g/mol]:</b>	124.22
<b>CAS:</b>	51708-83-9

## Physical Properties

Property code	Value	Unit	Source
gf	183.48	kJ/mol	Joback Method
hf	2.19	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	34.45	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	398.44	K	Joback Method
tc	574.80	K	Joback Method
tf	159.75	K	Joback Method
vc	0.503	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.07	J/molxK	398.44	Joback Method
cpg	255.62	J/molxK	427.83	Joback Method
cpg	268.57	J/molxK	457.23	Joback Method
cpg	280.95	J/molxK	486.62	Joback Method
cpg	292.78	J/molxK	516.01	Joback Method
cpg	304.07	J/molxK	545.40	Joback Method
cpg	314.85	J/molxK	574.80	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C51708839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51708839&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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