

# 2-Heptene, 4,6-dimethyl

<b>Inchi:</b>	InChI=1S/C9H18/c1-5-6-9(4)7-8(2)3/h5-6,8-9H,7H2,1-4H3/b6-5+
<b>InchiKey:</b>	TYWQCXCGSWSCFC-AATRIKPKSA-N
<b>Formula:</b>	C9H18
<b>SMILES:</b>	CC=CC(C)CC(C)C
<b>Mol. weight [g/mol]:</b>	126.24

## Physical Properties

Property code	Value	Unit	Source
gf	100.24	kJ/mol	Joback Method
hf	-122.43	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	34.81	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mvol	133.370	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rmpol	832.00		NIST Webbook
tb	408.60	K	Joback Method
tc	587.67	K	Joback Method
tf	156.11	K	Joback Method
vc	0.507	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.97	J/molxK	408.60	Joback Method
cpg	272.79	J/molxK	438.45	Joback Method
cpg	286.94	J/molxK	468.29	Joback Method
cpg	300.46	J/molxK	498.14	Joback Method
cpg	313.37	J/molxK	527.98	Joback Method
cpg	325.70	J/molxK	557.83	Joback Method
cpg	337.45	J/molxK	587.67	Joback Method
dvisc	0.0223846	Paxs	156.11	Joback Method
dvisc	0.0043187	Paxs	198.19	Joback Method

dvisc	0.0014827	Paxs	240.27	Joback Method
dvisc	0.0007001	Paxs	282.36	Joback Method
dvisc	0.0004016	Paxs	324.44	Joback Method
dvisc	0.0002618	Paxs	366.52	Joback Method
dvisc	0.0001863	Paxs	408.60	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R568280&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R568280&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>dvisc:</b>	Dynamic viscosity
<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>rinpol:</b>	Non-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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