

# 1,2-Hexadiene, 5-methyl-

<b>Inchi:</b>	InChI=1S/C7H12/c1-4-5-6-7(2)3/h5,7H,1,6H2,2-3H3
<b>InchiKey:</b>	NEYLAVKYYZDLIN-UHFFFAOYSA-N
<b>Formula:</b>	C7H12
<b>SMILES:</b>	C=C=CCC(C)C
<b>Mol. weight [g/mol]:</b>	96.17
<b>CAS:</b>	13865-36-6

## Physical Properties

Property code	Value	Unit	Source
gf	221.74	kJ/mol	Joback Method
hf	95.12	kJ/mol	Joback Method
hfus	11.21	kJ/mol	Joback Method
hvap	30.55	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.374		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	359.07	K	Joback Method
tc	541.60	K	Joback Method
tf	158.40	K	Joback Method
vc	0.383	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.03	J/molxK	359.07	Joback Method
cpg	183.53	J/molxK	389.49	Joback Method
cpg	193.66	J/molxK	419.91	Joback Method
cpg	203.43	J/molxK	450.33	Joback Method
cpg	212.84	J/molxK	480.75	Joback Method
cpg	221.91	J/molxK	511.17	Joback Method
cpg	230.63	J/molxK	541.60	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=C13865366&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13865366&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>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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