

# 2-Hexene, 3,5-dimethyl-

Inchi:	InChI=1S/C8H16/c1-5-8(4)6-7(2)3/h5,7H,6H2,1-4H3
InchiKey:	BQAZYKYBFAMHPG-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CC=C(C)CC(C)C
Mol. weight [g/mol]:	112.21
CAS:	3404-79-3

## Physical Properties

Property code	Value	Unit	Source
gf	85.71	kJ/mol	Joback Method
hf	-106.30	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	33.05	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	752.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	751.50		NIST Webbook
tb	386.04	K	Joback Method
tc	565.46	K	Joback Method
tf	145.88	K	Joback Method
vc	0.459	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/molxK	386.04	Joback Method
cpg	231.45	J/molxK	415.94	Joback Method
cpg	244.37	J/molxK	445.85	Joback Method
cpg	256.71	J/molxK	475.75	Joback Method
cpg	268.50	J/molxK	505.65	Joback Method
cpg	279.75	J/molxK	535.55	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404793&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404793&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>

## 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>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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