

# Hexenal, 3,5,5-trimethyl

<b>Inchi:</b>	InChI=1S/C9H16O/c1-8(5-6-10)7-9(2,3)4/h5-6H,7H2,1-4H3/b8-5+
<b>InchiKey:</b>	AQHLCHLIIMAFAA-VMPITWQZSA-N
<b>Formula:</b>	C9H16O
<b>SMILES:</b>	CC(=CC=O)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	140.22

## Physical Properties

Property code	Value	Unit	Source
gf	-0.11	kJ/mol	Joback Method
hf	-215.99	kJ/mol	Joback Method
hfus	12.83	kJ/mol	Joback Method
hvap	41.09	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpola	1046.00		NIST Webbook
tb	454.79	K	Joback Method
tc	647.33	K	Joback Method
tf	216.57	K	Joback Method
vc	0.526	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.01	J/mol×K	454.79	Joback Method
cpg	299.36	J/mol×K	486.88	Joback Method
cpg	312.88	J/mol×K	518.97	Joback Method
cpg	325.62	J/mol×K	551.06	Joback Method
cpg	337.60	J/mol×K	583.15	Joback Method
cpg	348.89	J/mol×K	615.24	Joback Method
cpg	359.52	J/mol×K	647.33	Joback Method

# Sources

<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=R90818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R90818&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>m cvol:</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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