

# 4-Methyl-2,4-pentadienal

<b>Inchi:</b>	InChI=1S/C6H8O/c1-6(2)4-3-5-7/h3-5H,1H2,2H3/b4-3+
<b>InchiKey:</b>	CPHXZIBGZOPWBM-ONEGZZNKSA-N
<b>Formula:</b>	C6H8O
<b>SMILES:</b>	C=C(C)C=CC=O
<b>Mol. weight [g/mol]:</b>	96.13

## Physical Properties

Property code	Value	Unit	Source
gf	59.63	kJ/mol	Joback Method
hf	-19.89	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.318		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpola	861.00		NIST Webbook
tb	386.06	K	Joback Method
tc	575.25	K	Joback Method
tf	178.58	K	Joback Method
vc	0.350	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.49	J/mol×K	386.06	Joback Method
cpg	159.43	J/mol×K	417.59	Joback Method
cpg	167.87	J/mol×K	449.12	Joback Method
cpg	175.85	J/mol×K	480.66	Joback Method
cpg	183.38	J/mol×K	512.19	Joback Method
cpg	190.48	J/mol×K	543.72	Joback Method
cpg	197.18	J/mol×K	575.25	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=R589470&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R589470&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccol:</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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