

# 2,4-Heptadienal, 2,4-dimethyl-

<b>Other names:</b>	2,4-Dimethyl-2,4-heptadienal
<b>Inchi:</b>	InChI=1S/C9H14O/c1-4-5-8(2)6-9(3)7-10/h5-7H,4H2,1-3H3/b8-5+,9-6+
<b>InchiKey:</b>	PHOBFHQBEYNKAL-XVYDYJIPSA-N
<b>Formula:</b>	C9H14O
<b>SMILES:</b>	CCC=C(C)C=C(C)C=O
<b>Mol. weight [g/mol]:</b>	138.21
<b>CAS:</b>	42452-48-2

## Physical Properties

Property code	Value	Unit	Source
gf	68.72	kJ/mol	Joback Method
hf	-99.81	kJ/mol	Joback Method
hfus	19.14	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.488		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	462.06	K	Joback Method
tc	655.30	K	Joback Method
tf	195.11	K	Joback Method
vc	0.518	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.06	J/molxK	462.06	Joback Method
cpg	278.99	J/molxK	494.27	Joback Method
cpg	291.21	J/molxK	526.47	Joback Method
cpg	302.74	J/molxK	558.68	Joback Method
cpg	313.64	J/molxK	590.88	Joback Method

cpg	323.93	J/mol×K	623.09	Joback Method
cpg	333.66	J/mol×K	655.30	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C42452482&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42452482&amp;Units=SI</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>mccvol:</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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