

# 1,5-Hexadien-3-ol, acetate

<b>Inchi:</b>	InChI=1S/C8H12O2/c1-4-6-8(5-2)10-7(3)9/h4-5,8H,1-2,6H2,3H3
<b>InchiKey:</b>	SUXVUJGA KOEPSL-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O2
<b>SMILES:</b>	C=CCC(C=C)OC(C)=O
<b>Mol. weight [g/mol]:</b>	140.18

## Physical Properties

Property code	Value	Unit	Source
gf	-44.20	kJ/mol	Joback Method
hf	-207.67	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	40.83	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.680		Crippen Method
mvol	122.420	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	901.00		NIST Webbook
tb	451.65	K	Joback Method
tc	637.95	K	Joback Method
tf	233.56	K	Joback Method
vc	0.464	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.76	J/molxK	451.65	Joback Method
cpg	258.10	J/molxK	482.70	Joback Method
cpg	268.95	J/molxK	513.75	Joback Method
cpg	279.33	J/molxK	544.80	Joback Method
cpg	289.24	J/molxK	575.85	Joback Method
cpg	298.70	J/molxK	606.90	Joback Method
cpg	307.71	J/molxK	637.95	Joback Method
dvisc	0.0038761	Paxs	233.56	Joback Method
dvisc	0.0017905	Paxs	269.91	Joback Method

dvisc	0.0009935	Paxs	306.26	Joback Method
dvisc	0.0006247	Paxs	342.61	Joback Method
dvisc	0.0004293	Paxs	378.95	Joback Method
dvisc	0.0003151	Paxs	415.30	Joback Method
dvisc	0.0002430	Paxs	451.65	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=U352718&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352718&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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