

# Acetic acid, 2-methylhex-3-yl ester

Inchi:	InChI=1S/C9H18O2/c1-5-6-9(7(2)3)11-8(4)10/h7,9H,5-6H2,1-4H3
InchiKey:	IUGAOCLNUASXDL-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCC(OC(C)=O)C(C)C
Mol. weight [g/mol]:	158.24

## Physical Properties

Property code	Value	Unit	Source
gf	-213.90	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1002.00		NIST Webbook
tb	480.73	K	Joback Method
tc	661.81	K	Joback Method
tf	233.35	K	Joback Method
vc	0.551	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.22	J/molxK	480.73	Joback Method
cpg	337.19	J/molxK	510.91	Joback Method
cpg	350.61	J/molxK	541.09	Joback Method
cpg	363.51	J/molxK	571.27	Joback Method
cpg	375.88	J/molxK	601.45	Joback Method
cpg	387.73	J/molxK	631.63	Joback Method
cpg	399.06	J/molxK	661.81	Joback Method
dvisc	0.0073761	Paxs	233.35	Joback Method
dvisc	0.0026314	Paxs	274.58	Joback Method

dvisc	0.0012286	Paxs	315.81	Joback Method
dvisc	0.0006840	Paxs	357.04	Joback Method
dvisc	0.0004299	Paxs	398.27	Joback Method
dvisc	0.0002948	Paxs	439.50	Joback Method
dvisc	0.0002156	Paxs	480.73	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=U368351&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368351&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>

## 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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