

# Acetoxyacetic acid, 3-methylbut-2-enyl ester

<b>Inchi:</b>	InChI=1S/C9H14O4/c1-7(2)4-5-12-9(11)6-13-8(3)10/h4H,5-6H2,1-3H3
<b>InchiKey:</b>	UABGOXKDESJTAT-UHFFFAOYSA-N
<b>Formula:</b>	C9H14O4
<b>SMILES:</b>	CC(=O)OCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	186.21

## Physical Properties

Property code	Value	Unit	Source
gf	-371.27	kJ/mol	Joback Method
hf	-611.26	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinqol	1252.00		NIST Webbook
tb	561.94	K	Joback Method
tc	754.41	K	Joback Method
tf	316.47	K	Joback Method
vc	0.569	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.59	J/molxK	561.94	Joback Method
cpg	360.64	J/molxK	594.02	Joback Method
cpg	372.16	J/molxK	626.10	Joback Method
cpg	383.14	J/molxK	658.17	Joback Method
cpg	393.58	J/molxK	690.25	Joback Method
cpg	403.50	J/molxK	722.33	Joback Method
cpg	412.90	J/molxK	754.41	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=U299203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299203&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>
<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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpolar:</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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