

# Acetic acid

# 5-ethoxy-2-ethoxymethyl-4-methoxy-tetrahydro-pyran-3-ester

InChI: CCOC(=O)C1OC(C)OC(C1)OC  
InChIKey: XOVGGTUZR VHREC-UHFFFAOYSA-N

Formula: C<sub>13</sub>H<sub>24</sub>O<sub>6</sub>

SMILES: CCOCC1OCC(OCC)C(OC)C1OC(C)=O

Mol. weight [g/mol]: 276.33

## Physical Properties

Property code	Value	Unit	Source
gf	-575.14	kJ/mol	Joback Method
hf	-1091.81	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.774		Crippen Method
mcvol	214.090	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1631.63		NIST Webbook
rinpol	1652.98		NIST Webbook
rinpol	1648.21		NIST Webbook
rinpol	1631.63		NIST Webbook
tb	672.88	K	Joback Method
tc	864.28	K	Joback Method
tf	396.35	K	Joback Method
vc	0.792	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.91	J/molxK	672.88	Joback Method
cpg	719.02	J/molxK	832.38	Joback Method
cpg	704.27	J/molxK	800.48	Joback Method
cpg	688.45	J/molxK	768.58	Joback Method
cpg	671.60	J/molxK	736.68	Joback Method
cpg	653.74	J/molxK	704.78	Joback Method

cpg	732.66	J/molxK	864.28	Joback Method
dvisc	0.0001357	Paxs	672.88	Joback Method
dvisc	0.0001667	Paxs	626.79	Joback Method
dvisc	0.0002114	Paxs	580.70	Joback Method
dvisc	0.0002793	Paxs	534.62	Joback Method
dvisc	0.0003890	Paxs	488.53	Joback Method
dvisc	0.0005805	Paxs	442.44	Joback Method
dvisc	0.0009507	Paxs	396.35	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=R262521&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R262521&amp;Units=SI</a>
<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>

## 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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