

# Acetoxyacetic acid, but-3-yn-2-yl ester

<b>Inchi:</b>	InChI=1S/C8H10O4/c1-4-6(2)12-8(10)5-11-7(3)9/h1,6H,5H2,2-3H3
<b>InchiKey:</b>	URQUXNXZRILLOT-UHFFFAOYSA-N
<b>Formula:</b>	C8H10O4
<b>SMILES:</b>	C#CC(C)OC(=O)COC(C)=O
<b>Mol. weight [g/mol]:</b>	170.16

## Physical Properties

Property code	Value	Unit	Source
gf	-230.73	kJ/mol	Joback Method
hf	-411.43	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Joback Method
hvap	51.18	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.114		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	524.70	K	Joback Method
tc	724.76	K	Joback Method
tf	356.21	K	Joback Method
vc	0.487	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.01	J/molxK	524.70	Joback Method
cpg	297.25	J/molxK	558.04	Joback Method
cpg	307.05	J/molxK	591.39	Joback Method
cpg	316.43	J/molxK	624.73	Joback Method
cpg	325.35	J/molxK	658.07	Joback Method
cpg	333.83	J/molxK	691.42	Joback Method
cpg	341.85	J/molxK	724.76	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=U299202&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299202&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>

# 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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