

# Ethyl 2-butynoate

<b>Other names:</b>	Ethyl tetrolate 2-Butynoic acid, ethyl ester Tetrolic acid, ethyl ester Ethyl 1-propynecarboxylate Ethyl 3-methylpropiolate
<b>Inchi:</b>	InChI=1S/C6H8O2/c1-3-5-6(7)8-4-2/h4H2,1-2H3
<b>InchiKey:</b>	FCJJZKCJURDYNF-UHFFFAOYSA-N
<b>Formula:</b>	C6H8O2
<b>SMILES:</b>	CC#CC(=O)OCC
<b>Mol. weight [g/mol]:</b>	112.13
<b>CAS:</b>	4341-76-8

## Physical Properties

Property code	Value	Unit	Source
gf	-31.48	kJ/mol	Joback Method
hf	-139.67	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.573		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	436.20	K	NIST Webbook
tc	625.16	K	Joback Method
tf	335.64	K	Joback Method
vc	0.357	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.07	J/molxK	421.97	Joback Method
cpg	180.45	J/molxK	455.84	Joback Method
cpg	188.58	J/molxK	489.70	Joback Method
cpg	196.44	J/molxK	523.57	Joback Method

cpg	204.02	J/mol×K	557.43	Joback Method
cpg	211.32	J/mol×K	591.30	Joback Method
cpg	218.34	J/mol×K	625.16	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	25.30	NIST Webbook

## 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=C4341768&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4341768&amp;Units=SI</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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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