

# Methyl 2-butynoate

<b>Other names:</b>	Methyl tetrolate 2-Butynoic acid, methyl ester
<b>Inchi:</b>	InChI=1S/C5H6O2/c1-3-4-5(6)7-2/h1-2H3
<b>InchiKey:</b>	UJQCANQILFWSDJ-UHFFFAOYSA-N
<b>Formula:</b>	C5H6O2
<b>SMILES:</b>	CC#CC(=O)OC
<b>Mol. weight [g/mol]:</b>	98.10
<b>CAS:</b>	23326-27-4

## Physical Properties

Property code	Value	Unit	Source
gf	-39.90	kJ/mol	Joback Method
hf	-119.03	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.183		Crippen Method
mvol	80.150	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	399.09	K	Joback Method
tc	604.33	K	Joback Method
tf	324.37	K	Joback Method
vc	0.301	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.16	J/molxK	399.09	Joback Method
cpg	143.89	J/molxK	433.30	Joback Method
cpg	150.45	J/molxK	467.50	Joback Method
cpg	156.83	J/molxK	501.71	Joback Method
cpg	163.02	J/molxK	535.92	Joback Method
cpg	169.01	J/molxK	570.12	Joback Method
cpg	174.80	J/molxK	604.33	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.70	K	11.00	NIST Webbook
tbrp	349.50 ± 0.50	K	11.00	NIST Webbook

## 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=C23326274&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23326274&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>

## 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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