

# 2-Butanone, 4-methoxy-

<b>Inchi:</b>	InChI=1S/C5H10O2/c1-5(6)3-4-7-2/h3-4H2,1-2H3
<b>InchiKey:</b>	DRWOJIXBYNGGW-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O2
<b>SMILES:</b>	COCCC(C)=O
<b>Mol. weight [g/mol]:</b>	102.13
<b>CAS:</b>	6975-85-5

## Physical Properties

Property code	Value	Unit	Source
gf	-242.70	kJ/mol	Joback Method
hf	-391.33	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	35.88	kJ/mol	Joback Method
ie	9.37	eV	NIST Webbook
log10ws	-0.28		Crippen Method
logp	0.612		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	390.09	K	Joback Method
tc	568.66	K	Joback Method
tf	218.27	K	Joback Method
vc	0.340	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.46	J/molxK	390.09	Joback Method
cpg	171.91	J/molxK	419.85	Joback Method
cpg	180.12	J/molxK	449.61	Joback Method
cpg	188.08	J/molxK	479.38	Joback Method
cpg	195.80	J/molxK	509.14	Joback Method
cpg	203.26	J/molxK	538.90	Joback Method
cpg	210.46	J/molxK	568.66	Joback Method
dvisc	0.0027914	Paxs	218.27	Joback Method

dvisc	0.0015155	Paxs	246.91	Joback Method
dvisc	0.0009341	Paxs	275.54	Joback Method
dvisc	0.0006307	Paxs	304.18	Joback Method
dvisc	0.0004556	Paxs	332.82	Joback Method
dvisc	0.0003466	Paxs	361.45	Joback Method
dvisc	0.0002744	Paxs	390.09	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=C6975855&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975855&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>ie:</b>	Ionization energy
<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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