

# 2-Butanone, 4-hydroxy-3-methyl-

<b>Other names:</b>	3-(Hydroxymethyl)-2-butanone 4-Hydroxy-3-methyl-2-butanone 4-hydroxy-3-methylbutan-2-one
<b>Inchi:</b>	InChI=1S/C5H10O2/c1-4(3-6)5(2)7/h4,6H,3H2,1-2H3
<b>InchiKey:</b>	VVSRECWZBBJOTG-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O2
<b>SMILES:</b>	CC(=O)C(C)CO
<b>Mol. weight [g/mol]:</b>	102.13
<b>CAS:</b>	3393-64-4

## Physical Properties

Property code	Value	Unit	Source
gf	-276.96	kJ/mol	Joback Method
hf	-416.62	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.204		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	826.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	826.00		NIST Webbook
tb	459.41	K	Joback Method
tc	635.76	K	Joback Method
tf	241.86	K	Joback Method
vc	0.335	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.97	J/molxK	606.37	Joback Method
cpg	227.44	J/molxK	635.76	Joback Method
cpg	183.94	J/molxK	459.41	Joback Method

cpg	191.99	J/molxK	488.80	Joback Method
cpg	199.72	J/molxK	518.19	Joback Method
cpg	207.12	J/molxK	547.58	Joback Method
cpg	214.20	J/molxK	576.97	Joback Method
dvisc	0.0002315	Paxs	459.41	Joback Method
dvisc	0.0003892	Paxs	423.15	Joback Method
dvisc	0.0540168	Paxs	241.86	Joback Method
dvisc	0.0120393	Paxs	278.12	Joback Method
dvisc	0.0037936	Paxs	314.38	Joback Method
dvisc	0.0015179	Paxs	350.63	Joback Method
dvisc	0.0007211	Paxs	386.89	Joback Method
hvapt	59.00	kJ/mol	387.50	NIST Webbook
hvapt	58.30	kJ/mol	451.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	2.00	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=C3393644&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3393644&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>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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</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>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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