

# Butanoic acid, 2-chloro-3-oxo-, methyl ester

<b>Other names:</b>	Methyl 2-chloroacetoacetate
<b>Inchi:</b>	InChI=1S/C5H7ClO3/c1-3(7)4(6)5(8)9-2/h4H,1-2H3
<b>InchiKey:</b>	GYQRIAVRKLRQKP-UHFFFAOYSA-N
<b>Formula:</b>	C5H7ClO3
<b>SMILES:</b>	COC(=O)C(Cl)C(C)=O
<b>Mol. weight [g/mol]:</b>	150.56
<b>CAS:</b>	4755-81-1

## Physical Properties

Property code	Value	Unit	Source
gf	-385.99	kJ/mol	Joback Method
hf	-524.93	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	0.356		Crippen Method
mcvol	102.560	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	410.20	K	NIST Webbook
tc	682.34	K	Joback Method
tf	283.12	K	Joback Method
vc	0.389	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.51	J/molxK	480.95	Joback Method
cpg	206.49	J/molxK	514.52	Joback Method
cpg	214.13	J/molxK	548.08	Joback Method
cpg	221.43	J/molxK	581.65	Joback Method
cpg	228.39	J/molxK	615.21	Joback Method
cpg	235.00	J/molxK	648.78	Joback Method
cpg	241.27	J/molxK	682.34	Joback Method
dvisc	0.0034472	Paxs	283.12	Joback Method

dvisc	0.0019084	Paxs	316.09	Joback Method
dvisc	0.0011814	Paxs	349.06	Joback Method
dvisc	0.0007945	Paxs	382.03	Joback Method
dvisc	0.0005690	Paxs	415.01	Joback Method
dvisc	0.0004281	Paxs	447.98	Joback Method
dvisc	0.0003349	Paxs	480.95	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4755811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4755811&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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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