

# Propanoic acid, 2-hydroxy-2-methyl-, methyl ester

<b>Other names:</b>	Methyl «alpha»-hydroxyisobutyrate Lactic acid, 2-methyl-, methyl ester Methyl 2-hydroxy-2-methylpropionate Methyl 2-hydroxyisobutyrate Methyl 2-methylactate Methyl ester of 2-methylactic acid 2-Hydroxyisobutyric acid, methyl ester
<b>Inchi:</b>	InChI=1S/C5H10O3/c1-5(2,7)4(6)8-3/h7H,1-3H3
<b>InchiKey:</b>	XYVQFUJDGOBPQI-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O3
<b>SMILES:</b>	COC(=O)C(C)(C)O
<b>Mol. weight [g/mol]:</b>	118.13
<b>CAS:</b>	2110-78-3

## Physical Properties

Property code	Value	Unit	Source
gf	-376.68	kJ/mol	Joback Method
hf	-552.31	kJ/mol	Joback Method
hfus	8.17	kJ/mol	Joback Method
hvap	51.26	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.070		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1116.00		NIST Webbook
tb	410.20	K	NIST Webbook
tc	661.63	K	Joback Method
tf	281.51	K	Joback Method
vc	0.347	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.95	J/mol×K	479.04	Joback Method
cpg	246.44	J/mol×K	631.20	Joback Method
cpg	239.51	J/mol×K	600.77	Joback Method
cpg	232.21	J/mol×K	570.34	Joback Method
cpg	224.53	J/mol×K	539.90	Joback Method
cpg	216.44	J/mol×K	509.47	Joback Method
cpg	253.01	J/mol×K	661.63	Joback Method
dvisc	0.0001875	Paxs	479.04	Joback Method
dvisc	0.0003027	Paxs	446.12	Joback Method
dvisc	0.0005275	Paxs	413.20	Joback Method
dvisc	0.0010120	Paxs	380.27	Joback Method
dvisc	0.0021967	Paxs	347.35	Joback Method
dvisc	0.0056086	Paxs	314.43	Joback Method
dvisc	0.0178299	Paxs	281.51	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2110783&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>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

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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