

# Pentanoic acid, 3-hydroxy-, methyl ester

<b>Other names:</b>	Methyl 3-hydroxypentanoate
<b>Inchi:</b>	InChI=1S/C6H12O3/c1-3-5(7)4-6(8)9-2/h5,7H,3-4H2,1-2H3
<b>InchiKey:</b>	XHFXXKFVUDJSPJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O3
<b>SMILES:</b>	CCC(O)CC(=O)OC
<b>Mol. weight [g/mol]:</b>	132.16
<b>CAS:</b>	56009-31-5

## Physical Properties

Property code	Value	Unit	Source
gf	-373.54	kJ/mol	Joback Method
hf	-569.48	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
ripol	1540.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	504.71	K	Joback Method
tc	679.05	K	Joback Method
tf	275.36	K	Joback Method
vc	0.408	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.76	J/molxK	504.71	Joback Method
cpg	254.84	J/molxK	533.77	Joback Method
cpg	263.60	J/molxK	562.82	Joback Method
cpg	272.02	J/molxK	591.88	Joback Method
cpg	280.10	J/molxK	620.94	Joback Method

cpg	287.86	J/molxK	649.99	Joback Method
cpg	295.29	J/molxK	679.05	Joback Method
dvisc	0.0210426	Paxs	275.36	Joback Method
dvisc	0.0055735	Paxs	313.59	Joback Method
dvisc	0.0019703	Paxs	351.81	Joback Method
dvisc	0.0008540	Paxs	390.03	Joback Method
dvisc	0.0004297	Paxs	428.26	Joback Method
dvisc	0.0002420	Paxs	466.49	Joback Method
dvisc	0.0001487	Paxs	504.71	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56009315&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56009315&amp;Units=SI</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>ripol:</b>	Polar retention indices
<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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