

# Butanoic acid, 3-hydroxy-, methyl ester

<b>Other names:</b>	Butyric acid, 3-hydroxy-, methyl ester Methyl 3-hydroxybutanoate Methyl «beta»-hydroxybutyrate Methyl 3-hydroxybutyrate CH3CH(OH)CH2C(O)OCH3 «beta»-Hydroxybutyric acid, methyl ester (.+/-)-3-Hydroxybutyric acid, methyl ester
<b>Inchi:</b>	InChI=1S/C5H10O3/c1-4(6)3-5(7)8-2/h4,6H,3H2,1-2H3
<b>InchiKey:</b>	LDLDJEAVRNAEBW-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O3
<b>SMILES:</b>	COC(=O)CC(C)O
<b>Mol. weight [g/mol]:</b>	118.13
<b>CAS:</b>	1487-49-6

## Physical Properties

Property code	Value	Unit	Source
gf	-381.96	kJ/mol	Joback Method
hf	-548.84	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.070		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	858.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	882.50		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	864.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1454.00		NIST Webbook

ripol	1475.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1465.00		NIST Webbook
tb	481.83	K	Joback Method
tc	657.66	K	Joback Method
tf	264.09	K	Joback Method
vc	0.352	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.80	J/molxK	481.83	Joback Method
cpg	212.77	J/molxK	511.13	Joback Method
cpg	220.46	J/molxK	540.44	Joback Method
cpg	227.87	J/molxK	569.74	Joback Method
cpg	235.00	J/molxK	599.05	Joback Method
cpg	241.86	J/molxK	628.35	Joback Method
cpg	248.43	J/molxK	657.66	Joback Method
dvisc	0.0255824	Paxs	264.09	Joback Method
dvisc	0.0067671	Paxs	300.38	Joback Method
dvisc	0.0023843	Paxs	336.67	Joback Method
dvisc	0.0010292	Paxs	372.96	Joback Method
dvisc	0.0005156	Paxs	409.25	Joback Method
dvisc	0.0002891	Paxs	445.54	Joback Method
dvisc	0.0001769	Paxs	481.83	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=C1487496&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1487496&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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>rinpol:</b>	Non-polar retention indices
<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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