

# Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester

<b>Other names:</b>	Vanillic acid, methyl ester Methyl vanillate Methyl 3-methoxy-4-hydroxybenzoate Methyl 4-hydroxy-3-methoxybenzoate 4-Hydroxy-3-methoxybenzoic acid methyl ester Methyl ester of 4-hydroxy-3-methoxybenzoic acid Vanillic acid methyl 4-Hydroxy-3-methoxybenzoic acid methyl ester (methyl vanillate)
<b>Inchi:</b>	InChI=1S/C9H10O4/c1-12-8-5-6(9(11)13-2)3-4-7(8)10/h3-5,10H,1-2H3
<b>InchiKey:</b>	BVWTXUYLKBHMOX-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O4
<b>SMILES:</b>	<chem>COC(=O)c1ccc(O)c(OC)c1</chem>
<b>Mol. weight [g/mol]:</b>	182.17
<b>CAS:</b>	3943-74-6

## Physical Properties

Property code	Value	Unit	Source
gf	-365.86	kJ/mol	Joback Method
hf	-558.36	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1516.90		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1527.00		NIST Webbook

ripol	2600.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2585.00		NIST Webbook
ripol	2580.00		NIST Webbook
ripol	2586.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2578.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2586.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2565.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2635.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2598.00		NIST Webbook
tb	559.20	K	NIST Webbook
tc	841.94	K	Joback Method
tf	436.24	K	Joback Method
vc	0.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/molxK	616.31	Joback Method
cpg	336.25	J/molxK	653.92	Joback Method
cpg	346.47	J/molxK	691.52	Joback Method
cpg	356.09	J/molxK	729.13	Joback Method
cpg	365.12	J/molxK	766.73	Joback Method
cpg	373.62	J/molxK	804.34	Joback Method
cpg	381.62	J/molxK	841.94	Joback Method
dvisc	0.0004335	Paxs	436.24	Joback Method
dvisc	0.0002352	Paxs	466.25	Joback Method

dvisc	0.0001374	Paxs	496.26	Joback Method
dvisc	0.0000854	Paxs	526.27	Joback Method
dvisc	0.0000558	Paxs	556.29	Joback Method
dvisc	0.0000381	Paxs	586.30	Joback Method
dvisc	0.0000270	Paxs	616.31	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=C3943746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3943746&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>	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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