

# Benzoic acid, 3,4-dihydroxy-, methyl ester

<b>Other names:</b>	Protocatechuic acid, methyl ester Methyl protocatechuate Methyl 3,4-dihydroxybenzoate 3,4-Dihydroxybenzoic acid methyl ester
<b>Inchi:</b>	InChI=1S/C8H8O4/c1-12-8(11)5-2-3-6(9)7(10)4-5/h2-4,9-10H,1H3
<b>InchiKey:</b>	CUFLZUDASVUNOE-UHFFFAOYSA-N
<b>Formula:</b>	C8H8O4
<b>SMILES:</b>	<chem>COC(=O)c1ccc(O)c(O)c1</chem>
<b>Mol. weight [g/mol]:</b>	168.15
<b>CAS:</b>	2150-43-8

## Physical Properties

Property code	Value	Unit	Source
gf	-414.27	kJ/mol	Joback Method
hf	-571.34	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.884		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
rinpol	1696.90		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	646.65	K	Joback Method
tc	888.33	K	Joback Method
tf	501.94	K	Joback Method
vc	0.332	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.69	J/mol×K	646.65	Joback Method
cpg	338.88	J/mol×K	848.05	Joback Method
cpg	331.74	J/mol×K	807.77	Joback Method

cpg	324.37	J/molxK	767.49	Joback Method
cpg	316.66	J/molxK	727.21	Joback Method
cpg	308.47	J/molxK	686.93	Joback Method
cpg	345.91	J/molxK	888.33	Joback Method
dvisc	0.0000038	Paxs	646.65	Joback Method
dvisc	0.0000055	Paxs	622.53	Joback Method
dvisc	0.0000084	Paxs	598.41	Joback Method
dvisc	0.0000133	Paxs	574.29	Joback Method
dvisc	0.0000218	Paxs	550.18	Joback Method
dvisc	0.0000375	Paxs	526.06	Joback Method
dvisc	0.0000678	Paxs	501.94	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2150438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2150438&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>rinpol:</b>	Non-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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