

# 2-Hydroxy-3-methoxybenzaldehyde, acetate

<b>Inchi:</b>	InChI=1S/C10H10O4/c1-7(12)14-10-8(6-11)4-3-5-9(10)13-2/h3-6H,1-2H3
<b>InchiKey:</b>	XRERBLZFFZMBKRU-UHFFFAOYSA-N
<b>Formula:</b>	C10H10O4
<b>SMILES:</b>	COc1cccc(C=O)c1OC(C)=O
<b>Mol. weight [g/mol]:</b>	194.18

## Physical Properties

Property code	Value	Unit	Source
gf	-311.97	kJ/mol	Joback Method
hf	-498.74	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.433		Crippen Method
mvol	142.880	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1522.90		NIST Webbook
rinpol	1522.90		NIST Webbook
tb	612.21	K	Joback Method
tc	827.41	K	Joback Method
tf	390.31	K	Joback Method
vc	0.546	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.79	J/molxK	612.21	Joback Method
cpg	350.19	J/molxK	648.08	Joback Method
cpg	360.97	J/molxK	683.94	Joback Method
cpg	371.12	J/molxK	719.81	Joback Method
cpg	380.62	J/molxK	755.68	Joback Method
cpg	389.47	J/molxK	791.54	Joback Method
cpg	397.65	J/molxK	827.41	Joback Method
dvisc	0.0011188	Paxs	390.31	Joback Method

dvisc	0.0007397	Paxs	427.29	Joback Method
dvisc	0.0005224	Paxs	464.28	Joback Method
dvisc	0.0003883	Paxs	501.26	Joback Method
dvisc	0.0003007	Paxs	538.24	Joback Method
dvisc	0.0002406	Paxs	575.23	Joback Method
dvisc	0.0001978	Paxs	612.21	Joback Method

## Sources

<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=U352859&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352859&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>

## 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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