

# 2-Propanone, 1-(4-hydroxy-2,6-dimethoxyphenyl)

Inchi:	InChI=1S/C11H14O4/c1-7(12)4-9-10(14-2)5-8(13)6-11(9)15-3/h5-6,13H,4H2,1-3H3
InchiKey:	PSOSBAWVFAPART-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COc1cc(O)cc(OC)c1CC(C)=O
Mol. weight [g/mol]:	210.23

## Physical Properties

Property code	Value	Unit	Source
gf	-358.65	kJ/mol	Joback Method
hf	-611.11	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.541		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpola	1707.00		NIST Webbook
rinpola	1707.00		NIST Webbook
tb	667.05	K	Joback Method
tc	885.56	K	Joback Method
tf	471.30	K	Joback Method
vc	0.551	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.53	J/molxK	667.05	Joback Method
cpg	475.62	J/molxK	849.14	Joback Method
cpg	465.83	J/molxK	812.72	Joback Method
cpg	455.46	J/molxK	776.31	Joback Method
cpg	444.47	J/molxK	739.89	Joback Method
cpg	432.84	J/molxK	703.47	Joback Method
cpg	484.86	J/molxK	885.56	Joback Method
dvisc	0.0000170	Paxs	667.05	Joback Method

dvisc	0.0000236	Paxs	634.42	Joback Method
dvisc	0.0000340	Paxs	601.80	Joback Method
dvisc	0.0000511	Paxs	569.17	Joback Method
dvisc	0.0000807	Paxs	536.55	Joback Method
dvisc	0.0001353	Paxs	503.93	Joback Method
dvisc	0.0002436	Paxs	471.30	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=R88386&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R88386&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>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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