

# Benzophenone, 5-chloro-2-hydroxy-4,4'-dimethoxy-

Inchi:	InChI=1S/C15H13ClO4/c1-19-10-5-3-9(4-6-10)15(18)11-7-12(16)14(20-2)8-13(11)17/h3-
InchiKey:	VDMMBVHCLKJIL-UHFFFAOYSA-N
Formula:	C15H13ClO4
SMILES:	COc1ccc(C(=O)c2cc(Cl)c(OC)cc2O)cc1
Mol. weight [g/mol]:	292.71
CAS:	136741-44-1

## Physical Properties

Property code	Value	Unit	Source
gf	-234.12	kJ/mol	Joback Method
hf	-484.35	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	84.49	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.294		Crippen Method
mcvol	206.110	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	827.66	K	Joback Method
tc	1073.00	K	Joback Method
tf	585.24	K	Joback Method
vc	0.717	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.08	J/molxK	827.66	Joback Method
cpg	570.96	J/molxK	868.55	Joback Method
cpg	581.99	J/molxK	909.44	Joback Method
cpg	592.24	J/molxK	950.33	Joback Method
cpg	601.77	J/molxK	991.22	Joback Method
cpg	610.66	J/molxK	1032.11	Joback Method
cpg	618.97	J/molxK	1073.00	Joback Method
dvisc	0.0000594	Paxs	585.24	Joback Method
dvisc	0.0000349	Paxs	625.64	Joback Method

dvisc	0.0000219	Paxs	666.05	Joback Method
dvisc	0.0000145	Paxs	706.45	Joback Method
dvisc	0.0000100	Paxs	746.85	Joback Method
dvisc	0.0000072	Paxs	787.26	Joback Method
dvisc	0.0000053	Paxs	827.66	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C136741441&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C136741441&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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