

# Chalcone, 2'-hydroxy-3',4,4',5',6'-pentamethoxy-

<b>Inchi:</b>	InChI=1S/C20H22O7/c1-23-13-9-6-12(7-10-13)8-11-14(21)15-16(22)18(25-3)20(27-5)19
<b>InchiKey:</b>	QRPYDMCAHJUWOJ-DHZHZOJOSA-N
<b>Formula:</b>	C20H22O7
<b>SMILES:</b>	COc1ccc(C=CC(=O)c2c(O)c(OC)c(OC)c(OC)c2OC)cc1
<b>Mol. weight [g/mol]:</b>	374.38
<b>CAS:</b>	50461-90-0

## Physical Properties

Property code	Value	Unit	Source
gf	-434.13	kJ/mol	Joback Method
hf	-874.19	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	99.74	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.331		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	3045.50		NIST Webbook
rinpol	3045.50		NIST Webbook
tb	986.01	K	Joback Method
tc	1220.07	K	Joback Method
tf	698.32	K	Joback Method
vc	0.982	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.75	J/molxK	986.01	Joback Method
cpg	879.90	J/molxK	1025.02	Joback Method
cpg	890.82	J/molxK	1064.03	Joback Method
cpg	900.54	J/molxK	1103.04	Joback Method
cpg	909.07	J/molxK	1142.05	Joback Method
cpg	916.43	J/molxK	1181.06	Joback Method
cpg	922.64	J/molxK	1220.07	Joback Method

dvisc	0.0000075	Paxs	698.32	Joback Method
dvisc	0.0000046	Paxs	746.27	Joback Method
dvisc	0.0000030	Paxs	794.22	Joback Method
dvisc	0.0000020	Paxs	842.17	Joback Method
dvisc	0.0000014	Paxs	890.11	Joback Method
dvisc	0.0000011	Paxs	938.06	Joback Method
dvisc	0.0000008	Paxs	986.01	Joback Method

## Sources

<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=C50461900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50461900&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>
<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>

## 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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