

# 5-Tert-butyl-2',4'-dichloro-2-hydroxybenzophenone

<b>Inchi:</b>	InChI=1S/C17H16Cl2O2/c1-17(2,3)10-4-7-15(20)13(8-10)16(21)12-6-5-11(18)9-14(12)19
<b>InchiKey:</b>	ZRPJXEAUDAUF0U-UHFFFAOYSA-N
<b>Formula:</b>	C17H16Cl2O2
<b>SMILES:</b>	CC(C)(C)c1ccc(O)c(C(=O)c2ccc(Cl)cc2Cl)c1
<b>Mol. weight [g/mol]:</b>	323.21
<b>CAS:</b>	61709-37-3

## Physical Properties

Property code	Value	Unit	Source
gf	-16.37	kJ/mol	Joback Method
hf	-285.68	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.228		Crippen Method
mcvol	234.790	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	862.78	K	Joback Method
tc	1119.96	K	Joback Method
tf	595.66	K	Joback Method
vc	0.831	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.66	J/molxK	862.78	Joback Method
cpg	700.05	J/molxK	1077.10	Joback Method
cpg	688.74	J/molxK	1034.23	Joback Method
cpg	677.34	J/molxK	991.37	Joback Method
cpg	665.64	J/molxK	948.51	Joback Method
cpg	653.47	J/molxK	905.64	Joback Method
cpg	711.42	J/molxK	1119.96	Joback Method
dvisc	0.0000045	Paxs	862.78	Joback Method
dvisc	0.0000062	Paxs	818.26	Joback Method

dvisc	0.0000089	Paxs	773.74	Joback Method
dvisc	0.0000134	Paxs	729.22	Joback Method
dvisc	0.0000212	Paxs	684.70	Joback Method
dvisc	0.0000359	Paxs	640.18	Joback Method
dvisc	0.0000656	Paxs	595.66	Joback Method

## Sources

<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=C61709373&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61709373&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>

## 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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