

# 4'-Chloro-2-hydroxy-5-t-octylbenzophenone

<b>Inchi:</b>	InChI=1S/C21H25ClO2/c1-4-5-6-13-21(2,3)16-9-12-19(23)18(14-16)20(24)15-7-10-17(22)
<b>InchiKey:</b>	OAOCLKRAKFBTQB-UHFFFAOYSA-N
<b>Formula:</b>	C21H25ClO2
<b>SMILES:</b>	CCCCC(C)(C)c1ccc(O)c(C(=O)c2ccc(Cl)cc2)c1
<b>Mol. weight [g/mol]:</b>	344.88

## Physical Properties

Property code	Value	Unit	Source
gf	38.87	kJ/mol	Joback Method
hf	-341.03	kJ/mol	Joback Method
hfus	41.61	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.135		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
tb	911.89	K	Joback Method
tc	1150.92	K	Joback Method
tf	598.30	K	Joback Method
vc	1.006	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.46	J/molxK	911.89	Joback Method
cpg	862.91	J/molxK	951.73	Joback Method
cpg	877.72	J/molxK	991.57	Joback Method
cpg	892.03	J/molxK	1031.40	Joback Method
cpg	906.03	J/molxK	1071.24	Joback Method
cpg	919.88	J/molxK	1111.08	Joback Method
cpg	933.75	J/molxK	1150.92	Joback Method
dvisc	0.0000570	Paxs	598.30	Joback Method
dvisc	0.0000275	Paxs	650.56	Joback Method
dvisc	0.0000148	Paxs	702.83	Joback Method

dvisc	0.0000087	Paxs	755.09	Joback Method
dvisc	0.0000054	Paxs	807.36	Joback Method
dvisc	0.0000036	Paxs	859.62	Joback Method
dvisc	0.0000025	Paxs	911.89	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=B6004170&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004170&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</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>hvac:</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>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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