

# Benzophenone, 5-heptyl-2,4-dihydroxy-

<b>Inchi:</b>	InChI=1S/C20H24O3/c1-2-3-4-5-7-12-16-13-17(19(22)14-18(16)21)20(23)15-10-8-6-9-1
<b>InchiKey:</b>	LHYZXFSSNRZNFV-UHFFFAOYSA-N
<b>Formula:</b>	C20H24O3
<b>SMILES:</b>	CCCCCCCc1cc(C(=O)c2ccccc2)c(O)cc1O
<b>Mol. weight [g/mol]:</b>	312.40
<b>CAS:</b>	116495-91-1

## Physical Properties

Property code	Value	Unit	Source
gf	-105.45	kJ/mol	Joback Method
hf	-461.74	kJ/mol	Joback Method
hfus	48.41	kJ/mol	Joback Method
hvap	98.10	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.842		Crippen Method
mcvol	258.450	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	930.45	K	Joback Method
tc	1167.18	K	Joback Method
tf	653.89	K	Joback Method
vc	0.877	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.46	J/molxK	930.45	Joback Method
cpg	895.50	J/molxK	1127.72	Joback Method
cpg	879.57	J/molxK	1088.27	Joback Method
cpg	863.99	J/molxK	1048.81	Joback Method
cpg	848.57	J/molxK	1009.36	Joback Method
cpg	833.12	J/molxK	969.90	Joback Method
cpg	911.97	J/molxK	1167.18	Joback Method
dvisc	0.0000002	Paxs	930.45	Joback Method
dvisc	0.0000002	Paxs	884.36	Joback Method

dvisc	0.0000004	Paxs	838.26	Joback Method
dvisc	0.0000006	Paxs	792.17	Joback Method
dvisc	0.0000012	Paxs	746.08	Joback Method
dvisc	0.0000022	Paxs	699.98	Joback Method
dvisc	0.0000047	Paxs	653.89	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=C116495911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495911&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>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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