

Benzophenone, 4'-chloro-2-hydroxy-4-methoxy-

Other names:	4'-chloro-2-hydroxy-4-methoxybenzophenone
Inchi:	InChI=1S/C14H11ClO3/c1-18-11-6-7-12(13(16)8-11)14(17)9-2-4-10(15)5-3-9/h2-8,16H,1
InchiKey:	CBKGNZGFDXQOEV-UHFFFAOYSA-N
Formula:	C14H11ClO3
SMILES:	COc1ccc(C(=O)c2ccc(Cl)cc2)c(O)c1
Mol. weight [g/mol]:	262.69
CAS:	85-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-127.91	kJ/mol	Joback Method
hf	-320.02	kJ/mol	Joback Method
hfus	32.09	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.285		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	777.38	K	Joback Method
tc	1030.73	K	Joback Method
tf	539.22	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.97	J/mol×K	777.38	Joback Method
cpg	494.71	J/mol×K	819.60	Joback Method
cpg	505.60	J/mol×K	861.83	Joback Method
cpg	515.76	J/mol×K	904.05	Joback Method
cpg	525.29	J/mol×K	946.28	Joback Method
cpg	534.30	J/mol×K	988.50	Joback Method
cpg	542.90	J/mol×K	1030.73	Joback Method
dvisc	0.0001293	Pa×s	539.22	Joback Method

dvisc	0.0000717	Pa×s	578.91	Joback Method
dvisc	0.0000428	Pa×s	618.61	Joback Method
dvisc	0.0000272	Pa×s	658.30	Joback Method
dvisc	0.0000182	Pa×s	697.99	Joback Method
dvisc	0.0000127	Pa×s	737.69	Joback Method
dvisc	0.0000092	Pa×s	777.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85289&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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