

2-Chloro-2'-hydroxy benzophenone

Inchi:	InChI=1S/C13H9ClO2/c14-11-7-3-1-5-9(11)13(16)10-6-2-4-8-12(10)15/h1-8,15H
InchiKey:	XKIZYRVSJNWVGM-UHFFFAOYSA-N
Formula:	C13H9ClO2
SMILES:	O=C(c1ccccc1O)c1ccccc1Cl
Mol. weight [g/mol]:	232.66
CAS:	70288-96-9

Physical Properties

Property code	Value	Unit	Source
gf	-21.70	kJ/mol	Joback Method
hf	-155.69	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.277		Crippen Method
mcvol	166.190	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	727.10	K	Joback Method
tc	990.16	K	Joback Method
tf	493.20	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.69	J/molxK	727.10	Joback Method
cpg	421.13	J/molxK	770.94	Joback Method
cpg	431.67	J/molxK	814.79	Joback Method
cpg	441.45	J/molxK	858.63	Joback Method
cpg	450.62	J/molxK	902.48	Joback Method
cpg	459.34	J/molxK	946.32	Joback Method
cpg	467.77	J/molxK	990.16	Joback Method
dvisc	0.0002993	Paxs	493.20	Joback Method
dvisc	0.0001539	Paxs	532.18	Joback Method

dvisc	0.0000866	Paxs	571.17	Joback Method
dvisc	0.0000525	Paxs	610.15	Joback Method
dvisc	0.0000338	Paxs	649.13	Joback Method
dvisc	0.0000228	Paxs	688.12	Joback Method
dvisc	0.0000161	Paxs	727.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C70288969&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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