(5-Chloro-2-hydroxyphenyl)(phenyl)methanone

Other names: Phenol, 2-benzoyl-4-chloro-
5-chloro-2-hydroxybenzophenone
Inchi: InChI=1S/C13H9ClO2/c14-10-6-7-12(15)11(8-10)13(16)9-4-2-1-3-5-9/h1-8,15H
InchiKey: OMWSZDODENFLSV-UHFFFAOYSA-N
Formula: C13H9ClO2
SMILES: O=C(c1ccccc1)c1cc(Cl)ccc1O
Mol. weight [g/mol]: 232.66
CAS: 85-19-8

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	459.34	J/mol×K	946.32	Joback Method
cpg	467.77	J/mol×K	990.16	Joback Method
cpg	409.69	J/mol×K	727.10	Joback Method
cpg	421.13	J/mol×K	770.94	Joback Method
cpg	431.67	J/mol×K	814.79	Joback Method
cpg	441.45	J/mol×K	858.63	Joback Method
cpg	450.62	J/mol×K	902.48	Joback Method

dvisc	0.0000161	Pa×s	727.10	Joback Method
dvisc	0.0000228	Pa×s	688.12	Joback Method
dvisc	0.0002993	Pa×s	493.20	Joback Method
dvisc	0.0001539	Pa×s	532.18	Joback Method
dvisc	0.0000866	Pa×s	571.17	Joback Method
dvisc	0.0000525	Pa×s	610.15	Joback Method
dvisc	0.0000338	Pa×s	649.13	Joback Method
hsubt	91.90	kJ/mol	330.00	NIST Webbook
hvapt	73.30	kJ/mol	430.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85198&Units=SI
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

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
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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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