Ethanone, 1-(5-chloro-2-hydroxyphenyl)-

Other names:	Acetophenone, 5'-chloro-2'-hydroxy-
	2-Acetyl-4-chlorophenol
	5'-Chloro-2'-hydroxyacetophenone
	2'-Hydroxy-5'-chloroacetophenone
	5-Chloro-2-hydroxyacetophenone
	1-(5-chloro-2-hydroxyphenyl)ethan-1-one
Inchi:	InChI=1S/C8H7ClO2/c1-5(10)7-4-6(9)2-3-8(7)11/h2-4,11H,1H3
InchiKey:	XTGCUDZCCIRWHL-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	CC(=O)c1cc(Cl)ccc1O
Mol. weight [g/mol]:	170.59
CAS:	1450-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-176.21	kJ/mol	Joback Method
hf	-289.02	kJ/mol	Joback Method
hfus	21.71	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.248		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
tb	586.02	K	Joback Method
tc	826.59	K	Joback Method
tf	410.43	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.23	J/mol×K	586.02	Joback Method
cpg	298.10	J/mol×K	786.50	Joback Method
cpg	291.23	J/mol×K	746.40	Joback Method

cpg	283.90	J/mol×K	706.31	Joback Method
cpg	276.01	J/mol×K	666.21	Joback Method
cpg	267.48	J/mol×K	626.12	Joback Method
cpg	304.58	J/mol×K	826.59	Joback Method
dvisc	0.0000530	Pa×s	586.02	Joback Method
dvisc	0.0000758	Pa×s	556.75	Joback Method
dvisc	0.0001126	Pa×s	527.49	Joback Method
dvisc	0.0001753	Pa×s	498.23	Joback Method
dvisc	0.0002884	Pa×s	468.96	Joback Method
dvisc	0.0005072	Pa×s	439.69	Joback Method
dvisc	0.0009664	Pa×s	410.43	Joback Method

Sources

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=C1450744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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