Acetophenone, 4'-hydroxy-

Other names:	1-(4-Hydroxyphenyl)ethanone 4'-hydroxyacetophenone 4-Hydroksyacetofenol 4-acetylphenol 4-hydroxyacetophenone 4-hydroxyphenyl methyl ketone Acetophenone, p-hydroxy- Ethanone, 1-(4-hydroxyphenyl)- Hydroxyacetophenone, para Methyl p-hydroxyphenyl ketone NSC 3698 Phenol, p-acetyl- Piceol USAF KF-15 p-Acetylphenol p-Hydroxyacetophenone p-Hydroxyphenyl methyl ketone p-Oxyacetophenone para-Hydroxyacetophenone phenol, 4-acetyl-
Inchi:	InChI=1S/C8H8O2/c1-6(9)7-2-4-8(10)5-3-7/h2-5,10H,1H3
InchiKey:	TXFPEBPIARQUIG-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	136.15
CAS:	99-93-4

Physical Properties

Property code	Value	Unit	Source
affp	883.70	kJ/mol	NIST Webbook
basg	851.90	kJ/mol	NIST Webbook
chs	-3927.10 ± 4.20	kJ/mol	NIST Webbook
gf	-154.65	kJ/mol	Joback Method
hf	-261.81	kJ/mol	Joback Method

hfus	17.03	kJ/mol	Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone
hvap	55.44	kJ/mol	Joback Method
ie	8.70 ± 0.03	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.595		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1490.70		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	543.61	K	Joback Method
tc	779.06	K	Joback Method
tf	379.65 ± 2.00	K	NIST Webbook
tf	311.00 ± 3.00	K	NIST Webbook
tf	383.00 ± 2.00	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.11	J/mol×K	700.57	Joback Method
cpg	289.93	J/mol×K	779.06	Joback Method
cpg	282.77	J/mol×K	739.81	Joback Method
cpg	237.80	J/mol×K	543.61	Joback Method
cpg	248.30	J/mol×K	582.85	Joback Method
cpg	257.96	J/mol×K	622.09	Joback Method
cpg	266.87	J/mol×K	661.33	Joback Method
dvisc	0.0000704	Pa×s	543.61	Joback Method
dvisc	0.0001656	Pa×s	485.07	Joback Method
dvisc	0.0001054	Pa×s	514.34	Joback Method
dvisc	0.0020779	Pa×s	367.99	Joback Method
dvisc	0.0009601	Pa×s	397.26	Joback Method
dvisc	0.0004932	Pa×s	426.53	Joback Method

dvisc	0.0002760	Pa×s	455.80	Joback Method
hfust	17.00	kJ/mol	381.30	NIST Webbook
hfust	18.08	kJ/mol	382.80	NIST Webbook
hsubt	95.70	kJ/mol	334.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.70	K	0.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, ortho/para-Hydroxyacetophenones and 4-hydroxyacetophenone:	https://www.doi.org/10.1016/j.fluid.2005.03.023
Solubility of 4-Hydroxyacetophenone in Aqueous Solutions of Sodium Alkyl Benzene Sulfonate Hydrotropes:	https://www.doi.org/10.1021/je034147s
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=C99934&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume