Ethanone, 1-(2-hydroxyphenyl)-

Other names:	1-(2-hydroxyphenyl)ethanone
	2'-hydroxyacetophenone
	2-Hydroxyacetylbenzene
	2-acetylphenol
	2-hydroxyphenyl methyl ketone
	Acetophenone, o-hydroxy-
	Methyl 2-hydroxyphenyl ketone
	NSC 16933
	USAF KE-20
	acetophenone, 2'-hydroxy-
	o-Acetylphenol
	o-Hydroxyacetophenone
	o-Hydroxyphenyl methyl ketone
	phenol, 2-acetyl-
Inchi:	InChI=1S/C8H8O2/c1-6(9)7-4-2-3-5-8(7)10/h2-5,10H,1H3
InchiKey:	JECYUBVRTQDVAT-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC(=O)c1ccccc1O
Mol. weight [g/mol]:	136.15
CAS:	118-93-4

Physical Properties

Property code	Value	Unit	Source
chs	-3933.80 ± 3.80	kJ/mol	NIST Webbook
ea	0.85 ± 0.05	eV	NIST Webbook
gf	-154.65	kJ/mol	Joback Method
hf	-261.81	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	58.30 ± 0.30	kJ/mol	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	1136.00		NIST Webbook
rinpol	1135.60		NIST Webbook
rinpol	1139.10		NIST Webbook
rinpol	1152.50		NIST Webbook

rinpol	1162.70		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1135.60		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1714.00		NIST Webbook
tb	491.20	K	NIST Webbook
tc	779.06	K	Joback Method
tf	301.15 ± 1.00	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.77	J/mol×K	739.81	Joback Method
cpg	289.93	J/mol×K	779.06	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
cpg	275.11	J/mol×K	700.57	Joback Method
dvisc	0.0000704	Pa×s	543.61	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
dvisc	0.0001656	Pa×s	485.07	Joback Method
hfust	13.00	kJ/mol	278.50	NIST Webbook
hvapt	58.30	kJ/mol	430.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	486.20	K	95.60	NIST Webbook
tbrp	379.20	K	2.30	NIST Webbook

Sources

Solubility of ortho/para-Hydroxyacetophenones 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=C118934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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
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