Ethanone, 1-(3-hydroxyphenyl)-

Other names:	1-(3-Hydroxyphenyl)ethan-1-one
	1-(3-hydroxyphenyl)ethanone
	3'-hydroxyacetophenone
	3-Hydroxyacetophenone
	3-acetylphenol
	3-hydroxyphenyl methyl ketone
	NSC 2440
	acetophenone, 3'-hydroxy-
	m-acetylphenol
	m-hydroxyacetophenone
	phenol, 3-acetyl-
Inchi:	InChI=1S/C8H8O2/c1-6(9)7-3-2-4-8(10)5-7/h2-5,10H,1H3
InchiKey:	LUJMEECXHPYQOF-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC(=O)c1cccc(O)c1
Mol. weight [g/mol]:	136.15
CAS:	121-71-1

Physical Properties

Property code	Value	Unit	Source
affp	863.60	kJ/mol	NIST Webbook
basg	831.80	kJ/mol	NIST Webbook
chs	-3920.80 ± 4.20	kJ/mol	NIST Webbook
gf	-154.65	kJ/mol	Joback Method
hf	-261.81	kJ/mol	Joback Method
hfus	23.36	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	8.67 ± 0.05	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	1358.10		NIST Webbook

rinpol	1438.50		NIST Webbook
rinpol	1358.10		NIST Webbook
tb	569.20	K	NIST Webbook
tc	779.06	K	Joback Method
tf	367.40 ± 2.00	K	NIST Webbook
tf	367.00 ± 3.00	K	NIST Webbook
tf	369.00 ± 3.00	K	NIST Webbook
tf	365.40 ± 2.00	K	NIST Webbook
tf	369.00 ± 2.00	K	NIST Webbook
tf	369.00 ± 4.00	K	NIST Webbook
tf	367.90 ± 2.00	K	NIST Webbook
tf	370.00 ± 2.00	K	NIST Webbook
tf	370.00 ± 2.00	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	282.77	J/mol×K	739.81	Joback Method
cpg	289.93	J/mol×K	779.06	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
dvisc	0.0001054	Pa×s	514.34	Joback Method
dvisc	0.0000704	Pa×s	543.61	Joback Method
hfust	23.40	kJ/mol	366.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	0.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121711&Units=SI
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, 3-hydroxyacetophenone and 4-hydroxyacetophenone:	https://www.doi.org/10.1016/j.fluid.2005.03.023
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume