

# Ethanone, 2-hydroxy-1-phenyl-

<b>Other names:</b>	Acetophenone, 2-hydroxy- «alpha»-Hydroxyacetophenone «omega»-Hydroxyacetophenone Benzoylcarbinol Glycolophenone Methanol, benzoyl- Phenacyl alcohol 2-Hydroxyacetophenone Hydroxymethyl phenyl ketone alpha-Hydroxyacetophenone Acetophenone, «alpha»-hydroxy- (Hydroxyacetyl)benzene NSC 171232 Acetophenone, alpha-hydroxy- 2-Hydroxy-phenylethanone 2-hydroxy-1-phenylethan-1-one
<b>Inchi:</b>	InChI=1S/C8H8O2/c9-6-8(10)7-4-2-1-3-5-7/h1-5,9H,6H2
<b>InchiKey:</b>	ZWVHTXAYIKBMEE-UHFFFAOYSA-N
<b>Formula:</b>	C8H8O2
<b>SMILES:</b>	O=C(CO)c1ccccc1
<b>Mol. weight [g/mol]:</b>	136.15
<b>CAS:</b>	582-24-1

## Physical Properties

Property code	Value	Unit	Source
gf	-136.85	kJ/mol	Joback Method
hf	-236.73	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
ie	9.33 ± 0.05	eV	NIST Webbook
log10ws	-1.40		Crippen Method
logp	0.862		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
ripol	1762.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1762.00		NIST Webbook

tb	555.17	K	Joback Method
tc	761.48	K	Joback Method
tf	317.09	K	Joback Method
vc	0.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.77	J/mol×K	555.17	Joback Method
cpg	278.92	J/mol×K	727.09	Joback Method
cpg	271.61	J/mol×K	692.71	Joback Method
cpg	263.77	J/mol×K	658.32	Joback Method
cpg	255.36	J/mol×K	623.94	Joback Method
cpg	246.37	J/mol×K	589.55	Joback Method
cpg	285.72	J/mol×K	761.48	Joback Method
dvisc	0.0001265	Paxs	555.17	Joback Method
dvisc	0.0001935	Paxs	515.49	Joback Method
dvisc	0.0003175	Paxs	475.81	Joback Method
dvisc	0.0005703	Paxs	436.13	Joback Method
dvisc	0.0011519	Paxs	396.45	Joback Method
dvisc	0.0027201	Paxs	356.77	Joback Method
dvisc	0.0079644	Paxs	317.09	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C582241&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C582241&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity

<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcpvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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