2-Hydroxyacetophenone

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

Physical Properties

Property code	Value	Unit	Source
af	0.6508		Cheméo Relay (1.0)
gf	-136.85	kJ/mol	Joback Method
hf	-243.05	kJ/mol	Cheméo Relay (1.0)
hfus	16.20	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Cheméo Relay (1.0)
ie	9.33 ± 0.05	eV	NIST Webbook
log10ws	-1.04		Cheméo Relay (1.0)
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	527.82	K	Cheméo Relay (1.0)
tc	783.43	K	Cheméo Relay (1.0)
tf	330.46	K	Cheméo Relay (1.0)
vc	0.380	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Effect of halogen substitution on the enthalpies of solvation and hydrogen bonding of organic solutes in chlorobenzene and 1,2-dichlorobenzene derived using multi-parameter correlations:	https://www.doi.org/10.1016/j.tca.2015.08.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C582241&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume