1-(4-Hydroxybenzylidene)acetone

Other names:	p-Hydroxybenzalacetone
	4-(p-Hydroxyphenyl)-3-buten-2-one
	4-Hydroxybenzylidene acetone
	3-Buten-2-one, 4-(4-hydroxyphenyl)-
	p-Hydroxybenzylidene acetone
	3-Buten-2-one, 4-(p-hydroxyphenyl)-
	4-Hydroxybenzalacetone
	4-(4-Hydroxyphenyl)-3-buten-2-one
	NSC 26516
	4-(4-hydroxyphenyl)but-3-en-2-one
Inchi:	InChI=1S/C10H10O2/c1-8(11)2-3-9-4-6-10(12)7-5-9/h2-7,12H,1H3/b3-2+
InchiKey:	OCNIKEFATSKIBE-NSCUHMNNSA-N
Formula:	C10H10O2
SMILES:	CC(=O)C=Cc1ccc(O)cc1
Mol. weight [g/mol]:	162.19
CAS:	3160-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-57.59	kJ/mol	Joback Method
hf	-185.87	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	59.85	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.994		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	593.53	K	Joback Method
tc	830.21	K	Joback Method
tf	385.45	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.69	J/mol×K	593.53	Joback Method
cpg	318.32	J/mol×K	632.98	Joback Method
cpg	329.04	J/mol×K	672.42	Joback Method
cpg	338.95	J/mol×K	711.87	Joback Method
cpg	348.17	J/mol×K	751.32	Joback Method
cpg	356.82	J/mol×K	790.76	Joback Method
cpg	365.00	J/mol×K	830.21	Joback Method
dvisc	0.0014544	Pa×s	385.45	Joback Method
dvisc	0.0006148	Pa×s	420.13	Joback Method
dvisc	0.0002964	Pa×s	454.81	Joback Method
dvisc	0.0001584	Pa×s	489.49	Joback Method
dvisc	0.0000920	Pa×s	524.17	Joback Method
dvisc	0.0000572	Pa×s	558.85	Joback Method
dvisc	0.0000375	Pa×s	593.53	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C3160358&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume