

1-Butanone, 1-(4-hydroxyphenyl)-

Other names:	1-(4-hydroxyphenyl)-1-butanone
	1-(4-hydroxyphenyl)butan-1-one
	4'-hydroxybutyrophenone
	4-Butanoylphenol
	4-Butyrylphenol
	4-Hydroxybutyrophenone
	Butyrophenone, 4'-hydroxy-
	NSC 17548
	p-Butyrylphenol
	p-Hydroxyphenyl propyl ketone
	p-hydroxybutyrophenone
Inchi:	InChI=1S/C10H12O2/c1-2-3-10(12)8-4-6-9(11)7-5-8/h4-7,11H,2-3H2,1H3
InchiKey:	GFBLPULLSAPXDC-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCCC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	164.20
CAS:	1009-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-137.81	kJ/mol	Joback Method
hf	-303.09	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.375		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	589.37	K	Joback Method
tc	815.81	K	Joback Method
tf	364.70	K	Thermochemistry of 4-HOC6H4COR (R = H, CH3, C2H5, n-C3H7, n-C4H9, n-C5H11, and n-C6H13) compounds
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.20	J/molxK	589.37	Joback Method
cpg	339.55	J/molxK	627.11	Joback Method
cpg	351.04	J/molxK	664.85	Joback Method
cpg	361.74	J/molxK	702.59	Joback Method
cpg	371.74	J/molxK	740.33	Joback Method
cpg	381.12	J/molxK	778.07	Joback Method
cpg	389.96	J/molxK	815.81	Joback Method
dvisc	0.0014890	Paxs	390.53	Joback Method
dvisc	0.0006624	Paxs	423.67	Joback Method
dvisc	0.0003314	Paxs	456.81	Joback Method
dvisc	0.0001821	Paxs	489.95	Joback Method
dvisc	0.0001079	Paxs	523.09	Joback Method
dvisc	0.0000681	Paxs	556.23	Joback Method
dvisc	0.0000452	Paxs	589.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1009116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of 4-HOC6H4COR (R = H, CH3, C2H5, n-C3H7, n-C4H9, n-C5H11, n-C6H13) compounds:	https://www.doi.org/10.1016/j.jct.2016.09.026
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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