1-Pentanone, 1-(4-hydroxyphenyl)-

Other names:	1-(4-hydroxyphenyl)-1-pentanone
	1-(4-hydroxyphenyl)pentan-1-one
	4'-hydroxyvalerophenone
	4-Valerylphenol
	Valerophenone, 4'-hydroxy-
	p-Valerylphenol
	p-hydroxyvalerophenone
Inchi:	InChI=1S/C11H14O2/c1-2-3-4-11(13)9-5-7-10(12)8-6-9/h5-8,12H,2-4H2,1H3
InchiKey:	ZKCJJGOOPOIZTE-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCCC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	178.23
CAS:	2589-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-129.39	kJ/mol	Joback Method
hf	-323.73	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.765		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	612.25	K	Joback Method
tc	834.48	K	Joback Method
tf	334.20	K	Thermochemistry of 4-HOC6H4COR (R = H, CH3, C2H5, n-C3H7, n-C4H9, n-C5H11, and n-C6H13) compounds
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	374.39	J/mol×K	612.25	Joback Method
cpg	387.50	J/mol×K	649.29	Joback Method
cpg	399.74	J/mol×K	686.33	Joback Method
cpg	411.18	J/mol×K	723.37	Joback Method
cpg	421.91	J/mol×K	760.40	Joback Method
cpg	432.01	J/mol×K	797.44	Joback Method
cpg	441.56	J/mol×K	834.48	Joback Method
dvisc	0.0012523	Pa×s	401.80	Joback Method
dvisc	0.0005477	Pa×s	436.88	Joback Method
dvisc	0.0002709	Pa×s	471.95	Joback Method
dvisc	0.0001477	Pa×s	507.02	Joback Method
dvisc	0.0000871	Pa×s	542.10	Joback Method
dvisc	0.0000548	Pa×s	577.17	Joback Method
dvisc	0.0000363	Pa×s	612.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.70	K	0.40	NIST Webbook

Sources

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, and n-C6H13) compounds:	https://www.doi.org/10.1016/j.jct.2016.09.026
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=C2589711&Units=SI

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