4-Hydroxy-2-methylacetophenone

Other names: 2-Methyl-4-hydroxyacetophenone
Ethanone, 1-(4-hydroxy-2-methylphenyl)-
Inchi: InChI=1S/C9H10O2/c1-6-5-8(11)3-4-9(6)7(2)10/h3-5,11H,1-2H3
InchiKey: IAMNVCJECQWBLZ-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: CC(=O)c1ccc(O)cc1C
Mol. weight [g/mol]: 150.17
CAS: 875-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-155.86	kJ/mol	Joback Method
hf	-293.92	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.903		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
ripol	1942.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1942.00		NIST Webbook
tb	586.20	K	NIST Webbook
tc	803.40	K	Joback Method
tf	391.78	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.73	J/mol×K	571.47	Joback Method
cpg	291.91	J/mol×K	610.13	Joback Method
cpg	302.30	J/mol×K	648.78	Joback Method
cpg	311.98	J/mol×K	687.44	Joback Method

cpg	321.02	J/mol×K	726.09	Joback Method
cpg	329.51	J/mol×K	764.75	Joback Method
cpg	337.51	J/mol×K	803.40	Joback Method
dvisc	0.0012185	Pa×s	391.78	Joback Method
dvisc	0.0006010	Pa×s	421.73	Joback Method
dvisc	0.0003256	Pa×s	451.68	Joback Method
dvisc	0.0001903	Pa×s	481.62	Joback Method
dvisc	0.0001185	Pa×s	511.57	Joback Method
dvisc	0.0000777	Pa×s	541.52	Joback Method
dvisc	0.0000533	Pa×s	571.47	Joback Method

Sources

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=C875592&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume