4-Hydroxy-3-methylacetophenone

Other names: 4'-Hydroxy-3'-methylacetophenone
Ethanone, 1-(4-hydroxy-3-methylphenyl)-
Inchi: InChI=1S/C9H10O2/c1-6-5-8(7(2)10)3-4-9(6)11/h3-5,11H,1-2H3
InchiKey: LXBHHIZIQVZGFN-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: CC(=O)c1ccc(O)c(C)c1
Mol. weight [g/mol]: 150.17
CAS: 876-02-8

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
rinpol	1323.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1322.00		NIST Webbook
ripol	2241.00		NIST Webbook
tb	571.47	K	Joback Method
tc	803.40	K	Joback Method
tf	382.00 ± 2.00	K	NIST Webbook
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	329.51	J/mol×K	764.75	Joback Method

cpg	321.02	J/mol×K	726.09	Joback Method
cpg	311.98	J/mol×K	687.44	Joback Method
cpg	302.30	J/mol×K	648.78	Joback Method
cpg	291.91	J/mol×K	610.13	Joback Method
cpg	337.51	J/mol×K	803.40	Joback Method
dvisc	0.0000533	Pa×s	571.47	Joback Method
dvisc	0.0000777	Pa×s	541.52	Joback Method
dvisc	0.0001185	Pa×s	511.57	Joback Method
dvisc	0.0001903	Pa×s	481.62	Joback Method
dvisc	0.0003256	Pa×s	451.68	Joback Method
dvisc	0.0006010	Pa×s	421.73	Joback Method
dvisc	0.0012185	Pa×s	391.78	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C876028&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume