Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-

Other names:	1-(2-Hydroxy-4-methoxyphenyl)-ethanone
	1-(2-hydroxy-4-methoxyphenyl)ethan-1-one
	2'-Hydroxy-4'-methoxyacetophenone
	2-Hydroxy-4-methoxyacetophenone
	2-Hydroxy-6-methoxybenzaldehyde
	Acetophenone, 2'-hydroxy-4'-methoxy-
	Paeonal
	Peonol
	Resacetophenone-4-methyl ether
	paeonol
Inchi:	InChI=1S/C9H10O3/c1-6(10)8-4-3-7(12-2)5-9(8)11/h3-5,11H,1-2H3
InchiKey:	UILPJVPSNHJFIK-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1ccc(C(C)=O)c(O)c1
Mol. weight [g/mol]:	166.17
CAS:	552-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-260.86	kJ/mol	Joback Method
hf	-426.14	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.603		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpol	1470.90		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1463.50		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1451.00		NIST Webbook
ripol	2300.00		NIST Webbook

ripol	2306.00		NIST Webbook
tb	593.89	K	Joback Method
tc	822.63	K	Joback Method
tf	414.01	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.95	J/mol×K	593.89	Joback Method
cpg	313.95	J/mol×K	632.01	Joback Method
cpg	324.24	J/mol×K	670.14	Joback Method
cpg	333.88	J/mol×K	708.26	Joback Method
cpg	342.92	J/mol×K	746.38	Joback Method
cpg	351.43	J/mol×K	784.51	Joback Method
cpg	359.45	J/mol×K	822.63	Joback Method
dvisc	0.0007214	Pa×s	414.01	Joback Method
dvisc	0.0003744	Pa×s	443.99	Joback Method
dvisc	0.0002111	Pa×s	473.97	Joback Method
dvisc	0.0001274	Pa×s	503.95	Joback Method
dvisc	0.0000814	Pa×s	533.93	Joback Method
dvisc	0.0000546	Pa×s	563.91	Joback Method
dvisc	0.0000381	Pa×s	593.89	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Measurement and Correlation of Paeonol Solubility in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/acs.jced.9b00483

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=C552410&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
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

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