

Ethanone, 1-(2-hydroxy-5-methoxyphenyl)-

Other names:	Acetophenone, 2'-hydroxy-5'-methoxy- 2-Hydroxy-5-methoxyacetophenone 2'-Hydroxy-5'-methoxyacetophenone 5-Methoxy-2-hydroxyacetophenone 1-(2-Hydroxy-5-methoxyphenyl)ethanone 1-(2-hydroxy-5-methoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C9H10O3/c1-6(10)8-5-7(12-2)3-4-9(8)11/h3-5,11H,1-2H3
InchiKey:	MLIBGOFSSXXWRIY-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1ccc(O)c(C(C)=O)c1
Mol. weight [g/mol]:	166.17
CAS:	705-15-7

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	1422.30		NIST Webbook
rinpol	1416.00		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/molxK	593.89	Joback Method

cpg	351.43	J/mol×K	784.51	Joback Method
cpg	342.92	J/mol×K	746.38	Joback Method
cpg	333.88	J/mol×K	708.26	Joback Method
cpg	324.24	J/mol×K	670.14	Joback Method
cpg	313.95	J/mol×K	632.01	Joback Method
cpg	359.45	J/mol×K	822.63	Joback Method
dvisc	0.0000381	Paxs	593.89	Joback Method
dvisc	0.0000546	Paxs	563.91	Joback Method
dvisc	0.0000814	Paxs	533.93	Joback Method
dvisc	0.0001274	Paxs	503.95	Joback Method
dvisc	0.0002111	Paxs	473.97	Joback Method
dvisc	0.0003744	Paxs	443.99	Joback Method
dvisc	0.0007214	Paxs	414.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C705157&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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