2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-

Other names:	Guaiacylacetone
	Vanillyl methyl ketone
	4-Hydroxy-3-methoxyphenyl acetone
	2-Propanone, (4-hydroxy-3-methoxyphenyl)-
	Methyl vanillyl ketone
	1-(4-Hydroxy-3-methoxy-phenyl)-propan-2-one
	1-(4-hydroxy-3-methoxyphenyl)-2-propanone
	2-Propiovanillone
	4-Hydroxy-3-methoxyphenylpropan-2-one
	Vanilloylmethyl ketone
	1-(4-Hydroxy-3-methoxyphenyl)-2-propanone (guaiacylacetone)
	1-(4-hydroxy-3-methoxyphenyl)acetone
Inchi:	InChI=1S/C10H12O3/c1-7(11)5-8-3-4-9(12)10(6-8)13-2/h3-4,6,12H,5H2,1-2H3
InchiKey:	LFVCJQWZGDLHSD-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1cc(CC(C)=O)ccc1O
Mol. weight [g/mol]:	180.20
CAS:	2503-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-252.44	kJ/mol	Joback Method
hf	-446.78	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.532		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	259.06		NIST Webbook
rinpol	1531.70		NIST Webbook
rinpol	1531.70		NIST Webbook

rinpol	1541.00		NIST Webbook
rinpol	1478.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
tb	616.77	K	Joback Method
tc	841.17	K	Joback Method
tf	425.28	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.42	J/mol×K	616.77	Joback Method
cpg	361.30	J/mol×K	654.17	Joback Method
cpg	372.44	J/mol×K	691.57	Joback Method
cpg	382.91	J/mol×K	728.97	Joback Method
cpg	392.75	J/mol×K	766.37	Joback Method
cpg	402.02	J/mol×K	803.77	Joback Method
cpg	410.79	J/mol×K	841.17	Joback Method
dvisc	0.0006184	Pa×s	425.28	Joback Method
dvisc	0.0003147	Pa×s	457.19	Joback Method
dvisc	0.0001749	Pa×s	489.11	Joback Method
dvisc	0.0001045	Pa×s	521.02	Joback Method
dvisc	0.0000662	Pa×s	552.94	Joback Method
dvisc	0.0000441	Pa×s	584.86	Joback Method
dvisc	0.0000307	Pa×s	616.77	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2503460&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume