Propiophenone, 4'-hydroxy-3'-methoxy

Other names:	1-(4-Hydroxy-3-methoxyphenyl)-1-propanone (propiovanillone)
	1-(4-hydroxy-3-methoxyphenyl)propanone
	1-(4-hydroxy-3-methoxyphenyl)propanone (propiovanillone)
	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)
	Propioguaiacone
	Propiophenone, 4'-hydroxy-3'-methoxy
Inchi:	InChI=1S/C10H12O3/c1-3-8(11)7-4-5-9(12)10(6-7)13-2/h4-6,12H,3H2,1-2H3
InchiKey:	FBGXENQFSMMBNY-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCC(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	180.20

Physical Properties

Property code	Value	Unit	Source
hf	-461.53	kJ/mol	Cheméo Relay (1.0)
hfus	23.88	kJ/mol	Joback Method
hvap	80.96	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-2.08		Cheméo Relay (1.0)
logp	1.993		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
tb	557.23	K	Cheméo Relay (1.0)
tf	388.43	K	Cheméo Relay (1.0)

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	457.20	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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1835149&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point