Propiovanillone

Other names:	Propioguaiacone
	1-(4-hydroxy-3-methoxyphenyl)propanone (propiovanillone)
	1-(4-Hydroxy-3-methoxyphenyl)-1-propanone (propiovanillone)
	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)
	1-(4-hydroxy-3-methoxyphenyl)propanone
	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
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	-2.22		Crippen Method
logp	1.994		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1529.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2693.00		NIST Webbook
ripol	2719.00		NIST Webbook
ripol	2677.00		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

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=C1835149&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