Ethanone, 1-(2,6-dihydroxy-4-methoxyphenyl)-

Other names:	Acetophenone, 2',6'-dihydroxy-4'-methoxy- 2,6-Dihydroxy-4-methoxyacetophenone 4-O-Methylphloracetophenone 1-(2,6-Dihydroxy-4-methoxyphenyl)ethanone Ethanone, 1-(2,6-hydroxy-4-methoxyphenyl)
Inchi:	InChI=1S/C9H10O4/c1-5(10)9-7(11)3-6(13-2)4-8(9)12/h3-4,11-12H,1-2H3
InchiKey:	GKSGTWUNURZTKD-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COc1cc(O)c(C(C)=O)c(O)c1
Mol. weight [g/mol]:	182.17
CAS:	7507-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-415.48	kJ/mol	Joback Method
hf	-603.45	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	73.75	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.309		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
rinpol	257.52		NIST Webbook
tb	674.51	K	Joback Method
tc	912.02	K	Joback Method
tf	525.73	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.94	J/mol×K	674.51	Joback Method
cpg	354.52	J/mol×K	714.10	Joback Method
cpg	363.55	J/mol×K	753.68	Joback Method

cpg	372.15	J/mol×K	793.27	Joback Method
cpg	380.44	J/mol×K	832.85	Joback Method
cpg	388.51	J/mol×K	872.44	Joback Method
cpg	396.49	J/mol×K	912.02	Joback Method
dvisc	0.0000400	Pa×s	525.73	Joback Method
dvisc	0.0000228	Pa×s	550.53	Joback Method
dvisc	0.0000137	Pa×s	575.32	Joback Method
dvisc	0.0000086	Pa×s	600.12	Joback Method
dvisc	0.0000056	Pa×s	624.92	Joback Method
dvisc	0.0000037	Pa×s	649.71	Joback Method
dvisc	0.0000026	Pa×s	674.51	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7507893&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