2,4'-Dihydroxy-3'-methoxyacetophenone

Other names:	2-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)ethanone
	Acetophenone, 2,4'-dihydroxy-3'-methoxy-
	Ethanone, 2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-
	Phenol, 4-hydroxyacetyl-2-methoxy-
Inchi:	InChI=1S/C9H10O4/c1-13-9-4-6(8(12)5-10)2-3-7(9)11/h2-4,10-11H,5H2,1H3
InchiKey:	QNMANLUEFQNQCX-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COc1cc(C(=O)CO)ccc1O
Mol. weight [g/mol]:	182.17
CAS:	18256-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-397.68	kJ/mol	Joback Method
hf	-578.37	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	0.576		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	686.07	K	Joback Method
tc	897.62	K	Joback Method
tf	474.83	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.80	J/mol×K	686.07	Joback Method
cpg	354.70	J/mol×K	721.33	Joback Method
cpg	363.09	J/mol×K	756.59	Joback Method
cpg	371.01	J/mol×K	791.85	Joback Method

cpg	378.51	J/mol×K	827.10	Joback Method
cpg	385.63	J/mol×K	862.36	Joback Method
cpg	392.42	J/mol×K	897.62	Joback Method
dvisc	0.0002480	Pa×s	474.83	Joback Method
dvisc	0.0001077	Pa×s	510.04	Joback Method
dvisc	0.0000520	Pa×s	545.24	Joback Method
dvisc	0.0000275	Pa×s	580.45	Joback Method
dvisc	0.0000156	Pa×s	615.66	Joback Method
dvisc	0.0000094	Pa×s	650.86	Joback Method
dvisc	0.0000060	Pa×s	686.07	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18256489&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume