2,5-Dihydroxypropiophenone

Other names:	2',5'-Dihydroxypropiophenone
	1-Propanone, 1-(2,5-dihydroxyphenyl)-
	Propiophenone, 2',5'-dihydroxy-
Inchi:	InChI=1S/C9H10O3/c1-2-8(11)7-5-6(10)3-4-9(7)12/h3-5,10,12H,2H2,1H3
InchiKey:	CFQYIIXIHXUPQT-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCC(=O)c1cc(O)ccc1O
Mol. weight [g/mol]:	166.17
CAS:	938-46-5

Physical Properties

Property code	Value	Unit	Source
gf	-300.85	kJ/mol	Joback Method
hf	-459.76	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	70.68	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.690		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	647.11	K	Joback Method
tc	887.44	K	Joback Method
tf	490.98	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.57	J/mol×K	647.11	Joback Method
cpg	334.36	J/mol×K	687.16	Joback Method
cpg	343.48	J/mol×K	727.22	Joback Method
cpg	352.06	J/mol×K	767.27	Joback Method
cpg	360.27	J/mol×K	807.33	Joback Method
cpg	368.23	J/mol×K	847.38	Joback Method

cpg	376.10	J/mol×K	887.44	Joback Method
dvisc	0.0001019	Pa×s	490.98	Joback Method
dvisc	0.0000525	Pa×s	517.00	Joback Method
dvisc	0.0000289	Pa×s	543.02	Joback Method
dvisc	0.0000167	Pa×s	569.05	Joback Method
dvisc	0.0000102	Pa×s	595.07	Joback Method
dvisc	0.0000065	Pa×s	621.09	Joback Method
dvisc	0.0000043	Pa×s	647.11	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C938465&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume