[1,1'-Biphenyl]-4,4'-diol, 3,3'-dimethoxy-

Other names:	4,4'-Biphenyldiol, 3,3'-dimethoxy-
	4,4'-Biguaiacol
	4,4'-Dihydroxy-3,3'-dimethoxybiphenyl
	1,1'-Biphenyl, 4,4'-dihydroxy-3,3'-dimethoxy
Inchi:	InChI=1S/C14H14O4/c1-17-13-7-9(3-5-11(13)15)10-4-6-12(16)14(8-10)18-2/h3-8,15-16H
InchiKey:	JJTJFVSZYDSLOT-UHFFFAOYSA-N
Formula:	C14H14O4
SMILES:	COc1cc(-c2ccc(O)c(OC)c2)ccc1O
Mol. weight [g/mol]:	246.26
CAS:	4433-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-246.68	kJ/mol	Joback Method
hf	-501.23	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.782		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	789.12	K	Joback Method
tc	1037.90	K	Joback Method
tf	593.32	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.56	J/mol×K	789.12	Joback Method
cpg	533.27	J/mol×K	830.58	Joback Method
cpg	545.37	J/mol×K	872.05	Joback Method
cpg	556.99	J/mol×K	913.51	Joback Method
cpg	568.28	J/mol×K	954.97	Joback Method

cpg	579.36	J/mol×K	996.44	Joback Method
cpg	590.37	J/mol×K	1037.90	Joback Method
dvisc	0.0000082	Pa×s	593.32	Joback Method
dvisc	0.0000045	Pa×s	625.95	Joback Method
dvisc	0.0000026	Pa×s	658.59	Joback Method
dvisc	0.0000016	Pa×s	691.22	Joback Method
dvisc	0.0000010	Pa×s	723.85	Joback Method
dvisc	0.0000007	Pa×s	756.49	Joback Method
dvisc	0.0000005	Pa×s	789.12	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=C4433094&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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