

4,4'-DIHYDROXY-3,3'-DIMETHOXYBIPHENYL

Other names:	1,1'-Biphenyl, 4,4'-dihydroxy-3,3'-dimethoxy 4,4'-Biguaiacol 4,4'-Biphenyldiol, 3,3'-dimethoxy- 4,4'-Dihydroxy-3,3'-dimethoxybiphenyl
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

Physical Properties

Property code	Value	Unit	Source
hf	-449.54	kJ/mol	Cheméo Relay (1.0)
hfus	33.26	kJ/mol	Joback Method
hvap	122.24	kJ/mol	Cheméo Relay (1.0)
ie	7.52	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	2.782		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
tb	629.59	K	Cheméo Relay (1.0)
tf	434.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.56	J/mol×K	789.12	Joback Method
cpg	590.37	J/mol×K	1037.90	Joback Method
cpg	579.36	J/mol×K	996.44	Joback Method
cpg	568.28	J/mol×K	954.97	Joback Method
cpg	556.99	J/mol×K	913.51	Joback Method
cpg	545.37	J/mol×K	872.05	Joback Method
cpg	533.27	J/mol×K	830.58	Joback Method
dvisc	0.0000016	Pa×s	691.22	Joback Method
dvisc	0.0000005	Pa×s	789.12	Joback Method

dvisc	0.0000007	Pa×s	756.49	Joback Method
dvisc	0.0000010	Pa×s	723.85	Joback Method
dvisc	0.0000082	Pa×s	593.32	Joback Method
dvisc	0.0000026	Pa×s	658.59	Joback Method
dvisc	0.0000045	Pa×s	625.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4433094&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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