3,3',5,5'-Tetramethoxy[1,1'-biphenyl]-4,4'-diol

Other names: 1,1'-Biphenyl, 3,3',5,5'-tetramethoxy-4,4'-dihydroxy
Inchi: InChI=1S/C16H18O6/c1-19-11-5-9(6-12(20-2)15(11)17)10-7-13(21-3)16(18)14(8-10)22-4
InchiKey: NRTOUGPMXLJETQ-UHFFFAOYSA-N
Formula: C16H18O6
SMILES: COc1cc(-c2cc(OC)c(O)c(OC)c2)cc(OC)c1O
Mol. weight [g/mol]: 306.31
CAS: 612-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-459.10	kJ/mol	Joback Method
hf	-829.89	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	94.08	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.799		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	889.68	K	Joback Method
tc	1126.17	K	Joback Method
tf	685.36	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.13	J/mol×K	889.68	Joback Method
cpg	692.32	J/mol×K	929.09	Joback Method
cpg	704.84	J/mol×K	968.51	Joback Method
cpg	716.76	J/mol×K	1007.92	Joback Method
cpg	728.15	J/mol×K	1047.34	Joback Method
cpg	739.06	J/mol×K	1086.75	Joback Method
cpg	749.57	J/mol×K	1126.17	Joback Method
dvisc	0.0000013	Pa×s	685.36	Joback Method

dvisc	0.0000008	Pa×s	719.41	Joback Method
dvisc	0.0000005	Pa×s	753.47	Joback Method
dvisc	0.0000003	Pa×s	787.52	Joback Method
dvisc	0.0000002	Pa×s	821.57	Joback Method
dvisc	0.0000002	Pa×s	855.63	Joback Method
dvisc	0.0000001	Pa×s	889.68	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=C612691&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