

2,2',6,6'-Tetramethyl-p,p'-biphenol

Other names:	[1,1'-Biphenyl]-4,4'-diol, 3,3',5,5'-tetramethyl-3,3',5,5'-Tetramethylbiphenyl-4,4'-diol
Inchi:	InChI=1S/C16H18O2/c1-9-5-13(6-10(2)15(9)17)14-7-11(3)16(18)12(4)8-14/h5-8,17-18H,
InchiKey:	YGYPMFPGZQPETF-UHFFFAOYSA-N
Formula:	C16H18O2
SMILES:	Cc1cc(-c2cc(C)c(O)c(C)c2)cc(C)c1O
Mol. weight [g/mol]:	242.31
CAS:	2417-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-39.10	kJ/mol	Joback Method
hf	-301.01	kJ/mol	Joback Method
hfus	35.29	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.998		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	800.00	K	Joback Method
tc	1047.82	K	Joback Method
tf	596.44	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.60	J/mol×K	800.00	Joback Method
cpg	588.88	J/mol×K	841.30	Joback Method
cpg	602.64	J/mol×K	882.61	Joback Method
cpg	616.06	J/mol×K	923.91	Joback Method
cpg	629.29	J/mol×K	965.21	Joback Method
cpg	642.50	J/mol×K	1006.51	Joback Method
cpg	655.87	J/mol×K	1047.82	Joback Method

dvisc	0.0000103	Pa×s	596.44	Joback Method
dvisc	0.0000056	Pa×s	630.37	Joback Method
dvisc	0.0000033	Pa×s	664.29	Joback Method
dvisc	0.0000020	Pa×s	698.22	Joback Method
dvisc	0.0000013	Pa×s	732.15	Joback Method
dvisc	0.0000009	Pa×s	766.07	Joback Method
dvisc	0.0000006	Pa×s	800.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2417041&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

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