Phenol, 4,4'-(1-methylethylidene)bis-

Other names:

2,2-(4',4''-dihydroxy)diphenylpropane
2,2-(4,4'-Dihydroxydiphenyl)propane
2,2-(4,4-Dihydroxydiphenyl)propane
2,2-Bis (4-hydroxyphenol) propane
2,2-Bis(4'-hydroxyphenyl)propane
2,2-Bis(4,4'-hydroxyphenyl)propane
2,2-Bis(4-hydroxyphenyl)propane
2,2-Bis(hydroxyphenyl)propane
2,2-Bis(p-hydroxyphenyl)propane
2,2-Bis-4'-hydroxyfenylpropan
2,2-Di(4-hydroxyphenyl)propane
2,2-Di(4-phenylol)propane
2,2-di-(4'-Hydroxyphenyl)-propane
2,2-di-(4-hydroxyphenyl)propane
4,4'-(1-METHYLETHYLIDENE)BIS-PHENOL
4,4'-(1-Methylethylidene)bisphenol
4,4'-(propane-2,2-diyl)diphenol
4,4'-Bisphenol A
4,4'-Dihydroxdiphenylpropane
4,4'-Dihydroxy-2,2-diphenylpropane
4,4'-Dihydroxydiphenyl-2,2-propane
4,4'-Dihydroxydiphenyldimethylmethane
4,4'-Dihydroxydiphenylpropane
4,4'-ISOPROPYLIDENEDI-PHENOL
4,4'-Isopropylidenebis[phenol]
4,4'-Isopropylidenediphenol
4,4-Isopropylidenediphenol
BPA 157
Biphenol A
Bis(4-hydroxyphenyl) dimethylmethane
Bis(p-hydroxyphenyl)propane
Bisferol A
Bisphenol
Bisphenol A
Dian
Diano
Dimethyl bis(p-hydroxyphenyl)methane
Dimethylmethylene-p,p'-diphenol
Diphenylolpropane
Ipognox 88

	Isopropylidenebis(4-hydroxybenzene)
	NCI-C50635
	Parabis
	Parabis A
	Phenol, (1-methylethylidene)bis-
	Phenol, 4,4'-dimethylmethylenedi-
	Phenol, 4,4'-isopropylidenedi-
	Pluracol 245
	Propane, 2,2-bis(p-hydroxyphenyl)-
	Rikabanol
	di-2,2-(4-Hydroxyphenyl)propane
	p,p'-Bisphenol A
	p,p'-Dihydroxydiphenyldimethylmethane
	p,p'-Dihydroxydiphenylpropane
	p,p'-Isopropylidenebisphenol
	p,p'-Isopropylidenediphenol
	«beta»,«beta»'-Bis(p-hydroxyphenyl)propane
	«beta»-di-p-hydroxyphenylpropane
	Â«betaÂ»,Â«betaÂ»'-Bis(p-hydroxyphenyl)propane
	Â«betaÂ»-di-p-hydroxyphenylpropane
Inchi:	InChI=1S/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1
InchiKey:	IISBACLAFKSPIT-UHFFFAOYSA-N
Formula:	C15H16O2
SMILES:	CC(C)(c1ccc(O)cc1)c1ccc(O)cc1
Mol. weight [g/mol]:	228.29
CAS:	80-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-6.16	kJ/mol	Joback Method
hf	-243.24	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Solubility of Bisphenol A in Supercritical Carbon Dioxide
hvap	78.27	kJ/mol	Joback Method
log10ws	-2.82		Aqueous Solubility Prediction Method
logp	3.424		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	2108.00		NIST Webbook

tb	753.97	K	Joback Method
tc	1018.62	K	Joback Method
tf	427.65	K	Aqueous Solubility Prediction Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.97	J/mol×K	753.97	Joback Method
cpg	543.20	J/mol×K	798.08	Joback Method
cpg	556.63	J/mol×K	842.19	Joback Method
cpg	569.54	J/mol×K	886.29	Joback Method
cpg	582.22	J/mol×K	930.40	Joback Method
cpg	594.96	J/mol×K	974.51	Joback Method
cpg	608.03	J/mol×K	1018.62	Joback Method
dvisc	0.0000313	Pa×s	537.51	Joback Method
dvisc	0.0000137	Pa×s	573.59	Joback Method
dvisc	0.0000066	Pa×s	609.66	Joback Method
dvisc	0.0000035	Pa×s	645.74	Joback Method
dvisc	0.0000019	Pa×s	681.82	Joback Method
dvisc	0.0000012	Pa×s	717.89	Joback Method
dvisc	0.0000007	Pa×s	753.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44248e+01
Coeff. B	-4.04412e+03
Coeff. C	-2.21266e+02
Temperature range (K), min.	507.33
Temperature range (K), max.	665.02

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.95077e+02
Coeff. B	-3.04193e+04
Coeff. C	-3.80451e+01
Coeff. D	7.42083e-06
Temperature range (K), min.	426.15
Temperature range (K), max.	849.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubilities of Estrone, 17p-Estradiol, 17a.-Ethynylestradiol, and Bisphenol A:	https://www.doi.org/10.1021/je050318c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol890.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80057&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=890
Solubility of Bisphenol A in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je200640q
The Solubility Behavior of Bisphenol A in the Presence of Surfactants:	https://www.doi.org/10.1021/je700235x

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume