Phenol, 2-[1-(4-hydroxyphenyl)-1-methylethyl]-

Other names: 2,4'-Bisphenol A
Phenol, 2-[1-(4-hydroxyphenyl)-1-methylethyl]-
2,4'-Dihydroxydiphenyldimethylmethane
2,4'-Isopropylidenediphenol
2-(4'-Hydroxyphenyl)-2-(2'-hydroxyphenyl)propane
o-[1-(4-hydroxyphenyl)-1-methylethyl]phenol

Inchi: InChI=1S/C15H16O2/c1-15(2,11-7-9-12(16)10-8-11)13-5-3-4-6-14(13)17/h3-10,16-17H,1

InchiKey: MLCQXUZZAXKTSG-UHFFFAOYSA-N

Formula: C15H16O2

SMILES: CC(C)(c1ccc(O)cc1)c1ccccc1O

Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
hf	-195.29	kJ/mol	Cheméo Relay (1.0)
hfus	26.84	kJ/mol	Joback Method
hvap	112.52	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	3.424		Crippen Method
mcvol	186.430	ml/mol	McGowan Method
tb	595.53	K	Cheméo Relay (1.0)
tf	372.42	K	Cheméo Relay (1.0)

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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C837081&Units=SI

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