4,4'-Dimethylbiphenyl

Other names:	1,1'-Biphenyl, 4,4'-dimethyl-
	1-Methyl-4-(4'-methylphenyl)benzene
	1-methyl-4-(4-methylphenyl)benzene
	4,4'-Bitolyl
	4,4'-Dimethyl-1,1'-biphenyl
	4,4'-Dimethyldiphenyl
	4,4'-Ditolyl
	Bi-p-tolyl
	Biphenyl, 4,4'-dimethyl-
	Di-p-tolyl
	Diphenyl, 4,4'-dimethyl
	NSC 90464
	p,p'-Bitoluene
	p,p'-Bitolyl
	p,p'-Ditolyl
Inchi:	InChI=1S/C14H14/c1-11-3-7-13(8-4-11)14-9-5-12(2)6-10-14/h3-10H,1-2H3
InchiKey:	RZTDESRVPFKCBH-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1ccc(-c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	182.26
CAS:	613-33-2

Physical Properties

Property code	Value	Unit	Source
chs	-7524.10 ± 7.50	kJ/mol	NIST Webbook
chs	-7526.10 ± 2.30	kJ/mol	NIST Webbook
gf	272.56	kJ/mol	Joback Method
hf	111.30 ± 3.60	kJ/mol	NIST Webbook
hfs	16.20 ± 2.90	kJ/mol	NIST Webbook
hfus	19.32	kJ/mol	Joback Method
hsub	95.10	kJ/mol	NIST Webbook
hsub	95.10 ± 2.00	kJ/mol	NIST Webbook
hsub	95.10 ± 2.00	kJ/mol	NIST Webbook
hvap	52.63	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-5.03		Crippen Method
logp	3.970		Crippen Method

mcvol	160.600	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1607.60		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1596.80		NIST Webbook
rinpol	1607.60		NIST Webbook
rinpol	1614.20		NIST Webbook
rinpol	277.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1614.20		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	277.49		NIST Webbook
rinpol	274.50		NIST Webbook
rinpol	274.50		NIST Webbook
rinpol	274.08		NIST Webbook
rinpol	274.59		NIST Webbook
rinpol	277.00		NIST Webbook
rinpol	274.44		NIST Webbook
rinpol	274.59		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1596.80		NIST Webbook
rinpol	1596.80		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1614.20		NIST Webbook
ripol	2236.00		NIST Webbook
ripol	2221.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2281.00		NIST Webbook
tb	562.00 ± 4.00	K	NIST Webbook
tb	569.00 ± 4.00	K	NIST Webbook
tb	568.00 ± 4.00	K	NIST Webbook
tb	568.20	K	NIST Webbook
tb	559.00 ± 5.00	K	NIST Webbook
tc	824.77	K	Joback Method
tf	395.00 ± 3.00	K	NIST Webbook
tf	355.00 ± 20.00	K	NIST Webbook
tf	393.00 ± 3.00	K	NIST Webbook
tf	394.10 ± 1.00	K	NIST Webbook
tf	392.70 ± 2.00	K	NIST Webbook
tf	394.00 ± 1.00	K	NIST Webbook
tf	392.90 ± 1.00	K	NIST Webbook

tf	394.00 ± 1.00	K	NIST Webbook
tf	394.00 ± 1.00	K	NIST Webbook
tf	396.00 ± 2.00	K	NIST Webbook
tf	393.00 ± 1.00	K	NIST Webbook
tf	391.70 ± 3.00	K	NIST Webbook
tf	394.70 ± 1.00	K	NIST Webbook
tf	393.70 ± 1.00	K	NIST Webbook
tf	395.00 ± 1.00	K	NIST Webbook
tf	394.70 ± 1.00	K	NIST Webbook
tf	391.00 ± 2.00	K	NIST Webbook
tf	391.00 ± 3.00	K	NIST Webbook
tf	392.70 ± 2.00	K	NIST Webbook
tf	394.00 ± 1.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	398.00 ± 2.00	K	NIST Webbook
tf	398.00 ± 2.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	395.00 ± 2.00	K	NIST Webbook
tf	395.70 ± 3.00	K	NIST Webbook
tf	394.00 ± 3.00	K	NIST Webbook
tf	394.00 ± 3.00	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	394.00 ± 3.00	K	NIST Webbook
tf	394.30 ± 1.50	K	NIST Webbook
tf	395.00 ± 4.00	K	NIST Webbook
tf	394.00 ± 3.00	K	NIST Webbook
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.50	J/mol×K	824.77	Joback Method
cpg	445.84	J/mol×K	784.48	Joback Method
cpg	433.22	J/mol×K	744.19	Joback Method
cpg	419.57	J/mol×K	703.90	Joback Method
cpg	404.83	J/mol×K	663.62	Joback Method
cpg	388.95	J/mol×K	623.33	Joback Method
cpg	371.85	J/mol×K	583.04	Joback Method
dvisc	0.0014925	Pa×s	325.42	Joback Method

dvisc	0.0001716	Pa×s	583.04	Joback Method
dvisc	0.0002132	Pa×s	540.10	Joback Method
dvisc	0.0002751	Pa×s	497.17	Joback Method
dvisc	0.0003724	Pa×s	454.23	Joback Method
dvisc	0.0005371	Pa×s	411.29	Joback Method
dvisc	0.0008435	Pa×s	368.36	Joback Method
hvapt	95.17	kJ/mol	298.15	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42880e+01
Coeff. B	-4.54144e+03
Coeff. C	-9.85400e+01
Temperature range (K), min.	422.92
Temperature range (K), max.	604.47

Sources

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=C613332&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls: https://www.doi.org/10.1016/j.fluid.2012.08.020

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume