1,1'-Biphenyl, 4-methyl-

Other names:	(4-Methylphenyl)benzene
	1-Methyl-4-phenylbenzene
	4-Methyl-1,1'-biphenyl
	4-Methylbiphenyl
	4-Methyldiphenyl
	4-Phenyltoluene
	Biphenyl, 4-methyl-
	FEMA 3186
	NSC 407669
	p-Methylbiphenyl
	p-Methyldiphenyl
	p-Phenyltoluene
Inchi:	InChI=1S/C13H12/c1-11-7-9-13(10-8-11)12-5-3-2-4-6-12/h2-10H,1H3
InchiKey:	ZZLCFHIKESPLTH-UHFFFAOYSA-N
Formula:	C13H12
SMILES:	Cc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	168.23
CAS:	644-08-6

Physical Properties

Property code	Value	Unit	Source
affp	817.90	kJ/mol	NIST Webbook
basg	785.40	kJ/mol	NIST Webbook
chs	-6888.60 ± 1.80	kJ/mol	NIST Webbook
chs	-6886.00 ± 7.10	kJ/mol	NIST Webbook
gf	273.77	kJ/mol	Joback Method
hf	138.20 ± 2.90	kJ/mol	NIST Webbook
hfs	58.00 ± 2.50	kJ/mol	NIST Webbook
hfus	12.29	kJ/mol	The heat capacities and thermodynamic functions of 4-methylbiphenyl and 4-tert-butylbiphenyl
hsub	80.20 ± 1.40	kJ/mol	NIST Webbook
hsub	80.20 ± 1.40	kJ/mol	NIST Webbook
hsub	80.20	kJ/mol	NIST Webbook
hvap	49.75	kJ/mol	Joback Method
ie	7.80 ± 0.02	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook

log10ws	-4.62		Estimated Solubility Method
log10ws	-4.62		Aqueous Solubility Prediction Method
logp	3.662		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1492.30		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1492.20		NIST Webbook
rinpol	257.30		NIST Webbook
rinpol	254.66		NIST Webbook
rinpol	256.00		NIST Webbook
rinpol	256.12		NIST Webbook
rinpol	256.69		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	255.90		NIST Webbook
rinpol	255.60		NIST Webbook
rinpol	256.70		NIST Webbook
rinpol	257.30		NIST Webbook
rinpol	254.71		NIST Webbook
rinpol	1492.20		NIST Webbook
rinpol	1482.80		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	255.90		NIST Webbook
rinpol	1497.30		NIST Webbook
rinpol	1492.20		NIST Webbook
rinpol	1482.80		NIST Webbook
rinpol	1497.30		NIST Webbook
rinpol	1492.20		NIST Webbook
rinpol	1482.80		NIST Webbook
rinpol	1492.30		NIST Webbook
rinpol	1492.20		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1484.50		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1472.70		NIST Webbook
rinpol	254.71		NIST Webbook
rinpol	1478.00		NIST Webbook

ripol	2182.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2134.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	547.50	K	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls
tc	800.99	K	Joback Method
tf	320.98	K	Aqueous Solubility Prediction Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.50	J/mol×K	555.18	Joback Method
cpg	341.24	J/mol×K	596.15	Joback Method
cpg	356.73	J/mol×K	637.12	Joback Method
cpg	371.02	J/mol×K	678.09	Joback Method
cpg	384.20	J/mol×K	719.06	Joback Method
cpg	396.32	J/mol×K	760.03	Joback Method
cpg	407.46	J/mol×K	800.99	Joback Method
dvisc	0.0019527	Pa×s	301.63	Joback Method
dvisc	0.0010384	Pa×s	343.89	Joback Method
dvisc	0.0006341	Pa×s	386.15	Joback Method
dvisc	0.0004268	Pa×s	428.40	Joback Method
dvisc	0.0003084	Pa×s	470.66	Joback Method
dvisc	0.0002351	Pa×s	512.92	Joback Method
dvisc	0.0001868	Pa×s	555.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45305e+01
Coeff. B	-4.44911e+03
Coeff. C	-9.21460e+01
Temperature range (K), min.	404.52
Temperature range (K), max.	574.75

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C644086&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls:	https://www.doi.org/10.1016/j.fluid.2012.08.020
Solubilities of p-Tolylboronic Acid, Bromobenzene and 4-Phenyltoluene in Carbon Dioxide at Elevated Pressures:	https://www.doi.org/10.1021/je034051y
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of 4-Phenyltoluene, Phenylboric Acid, Biphenyl, and 1,2-Dichlorobenzene in Carbon Dioxide from Measurements of the Relative Permittivity:	https://www.doi.org/10.1021/je050075o
The heat capacities and thermodynamic functions of 4-phenyl and 4-tert-butylbiphenyl :	https://www.doi.org/10.1016/j.jct.2010.05.002
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume