

1,1'-Biphenyl, 2-methyl-

Other names:	1-Methyl-2-phenylbenzene 2-Methyl-1,1'-biphenyl 2-Methylbiphenyl 2-Methyldiphenyl 2-Phenyltoluene Biphenyl, 2-methyl- o-Methylbiphenyl o-Phenyltoluene
Inchi:	InChI=1S/C13H12/c1-11-7-5-6-10-13(11)12-8-3-2-4-9-12/h2-10H,1H3
InchiKey:	ALLIZEAXNXSFGD-UHFFFAOYSA-N
Formula:	C13H12
SMILES:	<chem>Cc1ccccc1-c1ccccc1</chem>
Mol. weight [g/mol]:	168.23
CAS:	643-58-3

Physical Properties

Property code	Value	Unit	Source
affp	815.90	kJ/mol	NIST Webbook
basg	783.40	kJ/mol	NIST Webbook
chl	-6917.10 ± 1.20	kJ/mol	NIST Webbook
chl	-6950.90	kJ/mol	NIST Webbook
chl	-6694.00	kJ/mol	NIST Webbook
chl	-6938.70 ± 7.10	kJ/mol	NIST Webbook
gf	273.77	kJ/mol	Joback Method
hf	152.80 ± 1.50	kJ/mol	NIST Webbook
hfl	86.50 ± 1.30	kJ/mol	NIST Webbook
hfus	17.12	kJ/mol	Joback Method
hvap	66.30	kJ/mol	NIST Webbook
hvap	66.30 ± 0.50	kJ/mol	NIST Webbook
ie	8.10 ± 0.02	eV	NIST Webbook
log10ws	-4.55		Crippen Method
logp	3.662		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1402.30		NIST Webbook
rinpol	1390.00		NIST Webbook

rinpol	1397.60		NIST Webbook
rinpol	1397.60		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	255.70		NIST Webbook
rinpol	256.00		NIST Webbook
rinpol	1402.30		NIST Webbook
rinpol	239.57		NIST Webbook
rinpol	239.99		NIST Webbook
rinpol	240.00		NIST Webbook
rinpol	239.84		NIST Webbook
rinpol	238.55		NIST Webbook
rinpol	255.41		NIST Webbook
rinpol	238.77		NIST Webbook
rinpol	263.90		NIST Webbook
rinpol	238.20		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	263.90		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	238.77		NIST Webbook
rinpol	239.57		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	555.18	K	Joback Method
tc	800.99	K	Joback Method
tf	272.95 ± 0.15	K	NIST Webbook
tf	418.00	K	NIST Webbook
tf	272.95 ± 0.10	K	NIST Webbook
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.46	J/mol×K	800.99	Joback Method
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
dvisc	0.0001868	Pa×s	555.18	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
hvapt	65.23	kJ/mol	298.15	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41095e+01
Coeff. B	-4.21299e+03
Coeff. C	-8.81150e+01
Temperature range (K), min.	392.92
Temperature range (K), max.	566.97

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C643583&Units=SI>

The Yaws Handbook of Vapor

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
Study of critical and maximum temperatures of coexistence of liquid and gas phase in hydrocarbons binary mixtures of aromatic hydrocarbons with alkanes and cycloalkanes:
McGowan Method:

<https://www.doi.org/10.1016/j.fluid.2012.08.020>

<https://www.doi.org/10.1016/j.fluid.2014.06.020>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

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