

# 1,1'-Biphenyl, 2-(1-methylethyl)-

<b>Other names:</b>	1,1'-Biphenyl,2-isopropyl-
<b>Inchi:</b>	InChI=1S/C15H16/c1-12(2)14-10-6-7-11-15(14)13-8-4-3-5-9-13/h3-12H,1-2H3
<b>InchiKey:</b>	HKTCLPBBJDIBGF-UHFFFAOYSA-N
<b>Formula:</b>	C15H16
<b>SMILES:</b>	CC(C)c1ccccc1-c1ccccc1
<b>Mol. weight [g/mol]:</b>	196.29
<b>CAS:</b>	19486-60-3

## Physical Properties

Property code	Value	Unit	Source
chl	-7887.00	kJ/mol	NIST Webbook
gf	288.17	kJ/mol	Joback Method
hf	103.38	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
ie	8.50 ± 0.02	eV	NIST Webbook
log10ws	-5.26		Crippen Method
logp	4.477		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	2015.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	2015.00		NIST Webbook
tb	542.92 ± 0.15	K	NIST Webbook
tb	542.92 ± 0.30	K	NIST Webbook
tc	841.46	K	Joback Method
tf	297.61 ± 0.10	K	NIST Webbook
tf	297.61 ± 0.15	K	NIST Webbook
vc	0.653	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.76	J/molxK	600.50	Joback Method
cpg	501.11	J/molxK	801.30	Joback Method
cpg	487.65	J/molxK	761.14	Joback Method
cpg	473.06	J/molxK	720.98	Joback Method
cpg	457.26	J/molxK	680.82	Joback Method
cpg	440.19	J/molxK	640.66	Joback Method
cpg	513.52	J/molxK	841.46	Joback Method
dvisc	0.0001511	Paxs	600.50	Joback Method
dvisc	0.0001960	Paxs	551.95	Joback Method
dvisc	0.0002674	Paxs	503.39	Joback Method
dvisc	0.0003897	Paxs	454.84	Joback Method
dvisc	0.0006215	Paxs	406.28	Joback Method
dvisc	0.0011250	Paxs	357.73	Joback Method
dvisc	0.0024536	Paxs	309.17	Joback Method

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/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=C19486603&Units=SI>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure

<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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