

# 1,1'-Biphenyl, 2,2',5,5'-tetramethyl-

<b>Other names:</b>	2,2',5,5'-Tetramethyl-1,1'-biphenyl Biphenyl-, 2,2',5,5'-tetramethyl-
<b>Inchi:</b>	InChI=1S/C16H18/c1-11-5-7-13(3)15(9-11)16-10-12(2)6-8-14(16)4/h5-10H,1-4H3
<b>InchiKey:</b>	ZHTROMYSDSTCCE-UHFFFAOYSA-N
<b>Formula:</b>	C16H18
<b>SMILES:</b>	Cc1ccc(C)c(-c2cc(C)ccc2C)c1
<b>Mol. weight [g/mol]:</b>	210.31
<b>CAS:</b>	3075-84-1

## Physical Properties

Property code	Value	Unit	Source
gf	270.14	kJ/mol	Joback Method
hf	53.61	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.587		Crippen Method
mvol	188.780	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1668.50		NIST Webbook
rinpol	1663.60		NIST Webbook
rinpol	1663.20		NIST Webbook
rinpol	1656.50		NIST Webbook
tb	638.76	K	Joback Method
tc	872.54	K	Joback Method
tf	323.00 ± 4.00	K	NIST Webbook
tf	326.00 ± 4.00	K	NIST Webbook
vc	0.716	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.87	J/mol×K	638.76	Joback Method
cpg	548.43	J/mol×K	833.58	Joback Method

cpg	535.01	J/molxK	794.62	Joback Method
cpg	520.59	J/molxK	755.65	Joback Method
cpg	505.13	J/molxK	716.69	Joback Method
cpg	488.57	J/molxK	677.72	Joback Method
cpg	560.89	J/molxK	872.54	Joback Method
dvisc	0.0001447	Paxs	638.76	Joback Method
dvisc	0.0001759	Paxs	594.47	Joback Method
dvisc	0.0002209	Paxs	550.17	Joback Method
dvisc	0.0002885	Paxs	505.88	Joback Method
dvisc	0.0003967	Paxs	461.59	Joback Method
dvisc	0.0005836	Paxs	417.29	Joback Method
dvisc	0.0009410	Paxs	373.00	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	557.20	K	97.60	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29479e+01
Coeff. B	-4.05388e+03
Coeff. C	-9.63160e+01
Temperature range (K), min.	416.52
Temperature range (K), max.	627.18

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3075841&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/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>

## Legend

<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>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>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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