

# 3,3'-Di-tert-butylbiphenyl

<b>Inchi:</b>	InChI=1S/C20H26/c1-19(2,3)17-11-7-9-15(13-17)16-10-8-12-18(14-16)20(4,5)6/h7-14H,
<b>InchiKey:</b>	VBEKOHMKJMZVGZ-UHFFFAOYSA-N
<b>Formula:</b>	C20H26
<b>SMILES:</b>	CC(C)(C)c1cccc(-c2cccc(C(C)(C)C)c2)c1
<b>Mol. weight [g/mol]:</b>	266.42
<b>CAS:</b>	53692-24-3

## Physical Properties

Property code	Value	Unit	Source
gf	328.76	kJ/mol	Joback Method
hf	-23.51	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	63.40	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.949		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	713.86	K	Joback Method
tc	953.95	K	Joback Method
tf	397.88	K	Joback Method
vc	0.917	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.07	J/molxK	713.86	Joback Method
cpg	712.81	J/molxK	753.88	Joback Method
cpg	731.98	J/molxK	793.89	Joback Method
cpg	749.69	J/molxK	833.91	Joback Method
cpg	766.11	J/molxK	873.92	Joback Method
cpg	781.38	J/molxK	913.94	Joback Method
cpg	795.62	J/molxK	953.95	Joback Method
dvisc	0.0012913	Paxs	397.88	Joback Method
dvisc	0.0005947	Paxs	450.54	Joback Method

dvisc	0.0003222	Paxs	503.21	Joback Method
dvisc	0.0001960	Paxs	555.87	Joback Method
dvisc	0.0001300	Paxs	608.53	Joback Method
dvisc	0.0000920	Paxs	661.20	Joback Method
dvisc	0.0000685	Paxs	713.86	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53692243&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53692243&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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