

1,1'-Biphenyl, 3,3',4,4'-tetramethyl-

Other names:	Biphenyl, 3,3',4,4'-tetramethyl- 3,3',4,4'-Tetramethylbiphenyl 3,3',4,4'-Tetramethyldiphenyl 3,4,3',4'-Tetramethylbiphenyl
Inchi:	InChI=1S/C16H18/c1-11-5-7-15(9-13(11)3)16-8-6-12(2)14(4)10-16/h5-10H,1-4H3
InchiKey:	YXBIAZXZUDJVEB-UHFFFAOYSA-N
Formula:	C16H18
SMILES:	<chem>Cc1ccc(-c2ccc(C)c(C)c2)cc1C</chem>
Mol. weight [g/mol]:	210.31
CAS:	4920-95-0

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
mcvol	188.780	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
tb	638.76	K	Joback Method
tc	872.54	K	Joback Method
tf	349.00 ± 4.00	K	NIST Webbook
tf	349.00 ± 4.00	K	NIST Webbook
tf	350.00 ± 4.00	K	NIST Webbook
tf	350.00 ± 3.00	K	NIST Webbook
vc	0.716	m ³ /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/mol×K	794.62	Joback Method
cpg	520.59	J/mol×K	755.65	Joback Method
cpg	505.13	J/mol×K	716.69	Joback Method
cpg	488.57	J/mol×K	677.72	Joback Method
cpg	560.89	J/mol×K	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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4920950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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