3,3,'5,5'-Tetramethylbiphenyl

Other names:	1,1'-Biphenyl, 3,3',5,5'-tetramethyl-
	Biphenyl, 3,3',5,5'-tetramethyl-
	3,3',5,5'-Tetramethylbiphenyl
	2,2'5.5'-Tetramethylbiphenyl
Inchi:	InChI=1S/C16H18/c1-11-5-12(2)8-15(7-11)16-9-13(3)6-14(4)10-16/h5-10H,1-4H3
InchiKey:	CMZYGFLOKOQMKF-UHFFFAOYSA-N
Formula:	C16H18
SMILES:	Cc1cc(C)cc(-c2cc(C)cc(C)c2)c1
Mol. weight [g/mol]:	210.32

Physical Properties

Property code	Value	Unit	Source
af	0.5396		Cheméo Relay (1.0)
gf	270.14	kJ/mol	Joback Method
hf	65.76	kJ/mol	Cheméo Relay (1.0)
hfus	23.72	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Cheméo Relay (1.0)
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-6.56		Cheméo Relay (1.0)
logp	4.587		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
tb	587.19	K	Cheméo Relay (1.0)
tc	809.68	K	Cheméo Relay (1.0)
tf	322.00 ± 2.00	K	NIST Webbook
vc	0.724	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.87	J/mol×K	638.76	Joback Method
cpg	560.89	J/mol×K	872.54	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
dvisc	0.0002885	Pa×s	505.88	Joback Method
dvisc	0.0001447	Pa×s	638.76	Joback Method
dvisc	0.0001759	Pa×s	594.47	Joback Method
dvisc	0.0002209	Pa×s	550.17	Joback Method
dvisc	0.0009410	Pa×s	373.00	Joback Method
dvisc	0.0003967	Pa×s	461.59	Joback Method
dvisc	0.0005836	Pa×s	417.29	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25570029&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
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