3,3'-Dimethylbiphenyl

Other names:	1,1'-Biphenyl, 3,3'-dimethyl- 1-Methyl-3-(3'-methylphenyl)benzene 3,3'-Dimethyl-1,1'-biphenyl 3,3'-Dimethyldiphenyl 3,3'-Ditolyl 3,3-Dimethyldiphenyl Biphenyl, 3,3'-dimethyl- m,m'-Bitolyl
Inchi:	InChI=1S/C14H14/c1-11-5-3-7-13(9-11)14-8-4-6-12(2)10-14/h3-10H,1-2H3
InchiKey:	GVEDOIATHPCYGS-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1cccc(-c2cccc(C)c2)c1
Mol. weight [g/mol]:	182.26
CAS:	612-75-9

Physical Properties

Property code	Value	Unit	Source
chl	-7529.90 ± 7.50	kJ/mol	NIST Webbook
gf	272.56	kJ/mol	Joback Method
hf	117.83	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hsub	71.90	kJ/mol	NIST Webbook
hvap	71.90	kJ/mol	NIST Webbook
ie	7.85 ± 0.02	eV	NIST Webbook
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-5.03		Crippen Method
logp	3.970		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	271.87		NIST Webbook
rinpol	271.87		NIST Webbook
rinpol	270.79		NIST Webbook
rinpol	271.27		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1588.60		NIST Webbook

rinpol	1580.20		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1594.20		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	271.87		NIST Webbook
rinpol	1580.20		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1594.20		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1588.60		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2212.00		NIST Webbook
tb	559.00 ± 8.00	K	NIST Webbook
tb	561.00 ± 5.00	K	NIST Webbook
tb	559.00 ± 3.00	K	NIST Webbook
tb	556.00 ± 3.00	K	NIST Webbook
tb	562.00 ± 5.00	K	NIST Webbook
tc	824.77	K	Joback Method
tf	282.40 ± 1.50	K	NIST Webbook
tf	278.00 ± 3.00	K	NIST Webbook
tf	279.00 ± 3.00	K	NIST Webbook
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.85	J/mol×K	583.04	Joback Method
cpg	388.95	J/mol×K	623.33	Joback Method
cpg	404.83	J/mol×K	663.62	Joback Method
cpg	419.57	J/mol×K	703.90	Joback Method
cpg	433.22	J/mol×K	744.19	Joback Method
cpg	445.84	J/mol×K	784.48	Joback Method
cpg	457.50	J/mol×K	824.77	Joback Method
dvisc	0.0014925	Pa×s	325.42	Joback Method

dvisc	0.0008435	Pa×s	368.36	Joback Method
dvisc	0.0005371	Pa×s	411.29	Joback Method
dvisc	0.0003724	Pa×s	454.23	Joback Method
dvisc	0.0002751	Pa×s	497.17	Joback Method
dvisc	0.0002132	Pa×s	540.10	Joback Method
dvisc	0.0001716	Pa×s	583.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	559.20	K	95.10	NIST Webbook
tbrp	423.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44220e+01
Coeff. B	-4.53327e+03
Coeff. C	-9.65940e+01
Temperature range (K), min.	417.32
Temperature range (K), max.	594.18

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612759&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

chl:	Standard liquid enthalpy of combustion
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
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume