2,2'-Dimethylbiphenyl

Other names:	1,1'-Biphenyl, 2,2'-dimethyl-
	1-Methyl-2-(2'-methylphenyl)benzene
	2,2'-Bitolyl
	2,2'-Dimethyl-1,1'-biphenyl
	2,2'-Ditolyl
	Diphenyl, 2,2'-dimethyl
	O,O'-Bitoluene
	O,O'-Bitolyl
Inchi:	InChI=1S/C14H14/c1-11-7-3-5-9-13(11)14-10-6-4-8-12(14)2/h3-10H,1-2H3
InchiKey:	ABMKWMASVFVTMD-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1ccccc1-c1ccccc1C
Mol. weight [g/mol]:	182.26
CAS:	605-39-0

Physical Properties

Property code	Value	Unit	Source
gf	272.56	kJ/mol	Joback Method
hf	117.83	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
ie	8.05 ± 0.02	eV	NIST Webbook
ie	8.80 ± 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	261.78		NIST Webbook
rinpol	243.90		NIST Webbook
rinpol	241.94		NIST Webbook
rinpol	1546.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1950.00		NIST Webbook
sl	332.60	J/mol×K	NIST Webbook
tb	531.00 ± 4.00	K	NIST Webbook
tb	530.00 ± 4.00	K	NIST Webbook
tb	531.00 ± 4.00	K	NIST Webbook

tb	531.00 ± 3.00	K	NIST Webbook
tb	531.00 ± 4.00	K	NIST Webbook
tc	824.77	K	Joback Method
tf	325.42	K	Joback Method
tt	293.09 ± 0.01	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
cpl	298.06	J/mol×K	298.15	NIST Webbook
dvisc	0.0001716	Pa×s	583.04	Joback Method
dvisc	0.0008435	Pa×s	368.36	Joback Method
dvisc	0.0014925	Pa×s	325.42	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	0.0005371	Pa×s	411.29	Joback Method
hfust	2.28	kJ/mol	293.09	NIST Webbook
hfust	2.28	kJ/mol	293.10	NIST Webbook
hfust	2.28	kJ/mol	293.10	NIST Webbook
hsubt	65.70	kJ/mol	285.50	NIST Webbook
sfust	7.78	J/mol×K	293.09	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43603e+01
Coeff. B	-4.30779e+03

Coeff. C	-8.88100e+01
Temperature range (K), min.	394.92
Temperature range (K), max.	564.87

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C605390&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc: Critical Volume