

1,1'-Biphenyl, 3,4'-dimethyl-

Other names:	3,4'-Dimethyl-1,1'-biphenyl 3,4'-Dimethylbiphenyl 3,4'-Ditolyl 4,3'-Ditolyl Biphenyl, 3,4'-dimethyl- Diphenyl, 3,4'-dimethyl m,p'-Bitolyl
Inchi:	InChI=1S/C14H14/c1-11-6-8-13(9-7-11)14-5-3-4-12(2)10-14/h3-10H,1-2H3
InchiKey:	RBIDPZJTXXCPESJ-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1ccc(-c2cccc(C)c2)cc1
Mol. weight [g/mol]:	182.26
CAS:	7383-90-6

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
log10ws	-5.03		Crippen Method
logp	3.970		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1668.00		NIST Webbook
rinpol	1656.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2224.00		NIST Webbook
tb	559.00 ± 4.00	K	NIST Webbook
tb	569.00 ± 4.00	K	NIST Webbook
tc	824.77	K	Joback Method
tf	283.00 ± 4.00	K	NIST Webbook
tf	278.00 ± 5.00	K	NIST Webbook
tf	287.80 ± 0.60	K	NIST Webbook
tf	288.00 ± 3.00	K	NIST Webbook
tf	287.70 ± 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	426.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35890e+01
Coeff. B	-4.24527e+03
Coeff. C	-9.57600e+01
Temperature range (K), min.	414.92
Temperature range (K), max.	608.63

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7383906&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

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
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

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