

1,1'-Biphenyl, 2,6-dimethyl-

Inchi:	InChI=1S/C14H14/c1-11-7-6-8-12(2)14(11)13-9-4-3-5-10-13/h3-10H,1-2H3
InchiKey:	BGXRAGCQZCSMOT-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	Cc1cccc(C)c1-c1cccc1
Mol. weight [g/mol]:	182.26
CAS:	3976-34-9

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	1465.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1465.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1983.00		NIST Webbook
tb	535.70	K	NIST Webbook
tb	536.00 ± 5.00	K	NIST Webbook
tc	824.77	K	Joback Method
tf	268.00 ± 3.00	K	NIST Webbook
vc	0.604	m ³ /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/molxK	703.90	Joback Method
cpg	433.22	J/molxK	744.19	Joback Method
cpg	445.84	J/molxK	784.48	Joback Method
cpg	457.50	J/molxK	824.77	Joback Method
dvisc	0.0014925	Paxs	325.42	Joback Method
dvisc	0.0008435	Paxs	368.36	Joback Method
dvisc	0.0005371	Paxs	411.29	Joback Method
dvisc	0.0003724	Paxs	454.23	Joback Method
dvisc	0.0002751	Paxs	497.17	Joback Method
dvisc	0.0002132	Paxs	540.10	Joback Method
dvisc	0.0001716	Paxs	583.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	2.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3976349&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

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
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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