

1,1'-Biphenyl-3-ol, 4'-chloro

Inchi:	InChI=1S/C12H9ClO/c13-11-6-4-9(5-7-11)10-2-1-3-12(14)8-10/h1-8,14H
InchiKey:	CIPDQYWUAVNLSD-UHFFFAOYSA-N
Formula:	C12H9ClO
SMILES:	Oc1cccc(-c2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	204.65

Physical Properties

Property code	Value	Unit	Source
gf	98.80	kJ/mol	Joback Method
hf	-22.47	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.713		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook
tb	650.35	K	Joback Method
tc	914.63	K	Joback Method
tf	432.00	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.29	J/mol×K	650.35	Joback Method
cpg	363.75	J/mol×K	694.40	Joback Method
cpg	375.13	J/mol×K	738.44	Joback Method
cpg	385.60	J/mol×K	782.49	Joback Method
cpg	395.30	J/mol×K	826.54	Joback Method
cpg	404.39	J/mol×K	870.58	Joback Method
cpg	413.02	J/mol×K	914.63	Joback Method

dvisc	0.0006154	Pa×s	432.00	Joback Method
dvisc	0.0002923	Pa×s	468.39	Joback Method
dvisc	0.0001545	Pa×s	504.78	Joback Method
dvisc	0.0000890	Pa×s	541.17	Joback Method
dvisc	0.0000550	Pa×s	577.57	Joback Method
dvisc	0.0000359	Pa×s	613.96	Joback Method
dvisc	0.0000246	Pa×s	650.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R343056&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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