

1,1'-Biphenyl-3-ol, 2'-chloro

Inchi:	InChI=1S/C12H9ClO/c13-12-7-2-1-6-11(12)9-4-3-5-10(14)8-9/h1-8,14H
InchiKey:	YQFPFQICZVMDML-UHFFFAOYSA-N
Formula:	C12H9ClO
SMILES:	Oc1cccc(-c2ccccc2Cl)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
mvol	150.530	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	650.35	K	Joback Method
tc	914.63	K	Joback Method
tf	432.00	K	Joback Method
vc	0.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.29	J/molxK	650.35	Joback Method
cpg	363.75	J/molxK	694.40	Joback Method
cpg	375.13	J/molxK	738.44	Joback Method
cpg	385.60	J/molxK	782.49	Joback Method
cpg	395.30	J/molxK	826.54	Joback Method
cpg	404.39	J/molxK	870.58	Joback Method
cpg	413.02	J/molxK	914.63	Joback Method
dvisc	0.0006154	Paxs	432.00	Joback Method

dvisc	0.0002923	Paxs	468.39	Joback Method
dvisc	0.0001545	Paxs	504.78	Joback Method
dvisc	0.0000890	Paxs	541.17	Joback Method
dvisc	0.0000550	Paxs	577.57	Joback Method
dvisc	0.0000359	Paxs	613.96	Joback Method
dvisc	0.0000246	Paxs	650.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R343536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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