

[1,1'-Biphenyl-3-ol], 6-chloro-

Inchi:	InChI=1S/C12H9ClO/c13-12-7-6-10(14)8-11(12)9-4-2-1-3-5-9/h1-8,14H
InchiKey:	UGRROGFBORDDFR-UHFFFAOYSA-N
Formula:	C12H9ClO
SMILES:	Oc1ccc(Cl)c(-c2ccccc2)c1
Mol. weight [g/mol]:	204.65
CAS:	21345-13-1

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	1728.00		NIST Webbook
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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/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	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

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=C21345131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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