

1,1'-Biphenyl-3-ol, 2,4'-dichloro

Inchi:	InChI=1S/C12H8Cl2O/c13-9-6-4-8(5-7-9)10-2-1-3-11(15)12(10)14/h1-7,15H
InchiKey:	QRRCV FHAGKYXRZ-UHFFFAOYSA-N
Formula:	C12H8Cl2O
SMILES:	Oc1cccc(-c2ccc(Cl)cc2)c1Cl
Mol. weight [g/mol]:	239.10

Physical Properties

Property code	Value	Unit	Source
gf	77.24	kJ/mol	Joback Method
hf	-49.68	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.366		Crippen Method
mcvol	162.770	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	692.76	K	Joback Method
tc	960.07	K	Joback Method
tf	474.44	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.08	J/molxK	692.76	Joback Method
cpg	382.17	J/molxK	737.31	Joback Method
cpg	392.36	J/molxK	781.86	Joback Method
cpg	401.79	J/molxK	826.42	Joback Method
cpg	410.63	J/molxK	870.97	Joback Method
cpg	419.03	J/molxK	915.52	Joback Method
cpg	427.12	J/molxK	960.07	Joback Method

dvisc	0.0003217	Paxs	474.44	Joback Method
dvisc	0.0001697	Paxs	510.83	Joback Method
dvisc	0.0000975	Paxs	547.21	Joback Method
dvisc	0.0000600	Paxs	583.60	Joback Method
dvisc	0.0000391	Paxs	619.99	Joback Method
dvisc	0.0000267	Paxs	656.37	Joback Method
dvisc	0.0000190	Paxs	692.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R343001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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