

# [1,1'-Biphenyl]-4,4'-diamine, 3,3'-dichloro-

<b>Other names:</b>	3,3'-Dichlorbenzidin 3,3'-Dichloro-1,1'-biphenyl-4,4'-diamine 3,3'-Dichloro-4,4'-biphenyldiamine 3,3'-Dichloro-4,4'-diamino(1,1-biphenyl) 3,3'-Dichloro-4,4'-diaminobiphenyl 3,3'-Dichloro-4,4'-diaminodiphenyl 3,3'-Dichloro-p,p'-bianiline 3,3'-Dichlorobenzidina 3,3'-Dichlorobenzidine 3,3'-Dichlorobiphenyl-4,4'-diamine 3,3'-dichlorobiphenyl-4,4'-ylenediamine 4,4'-Diamino-3,3'-dichlorobiphenyl 4,4'-Diamino-3,3'-dichlorodiphenyl 4-(4-amino-3-chlorophenyl)-2-chloroaniline Benzidine, 3,3'-dichloro- C.I. 23060 Curithane C 126 Dichlorobenzidine base NSC 154073 Rcra waste number U073 o,o'-Dichlorobenzidine
<b>Inchi:</b>	InChI=1S/C12H10Cl2N2/c13-9-5-7(1-3-11(9)15)8-2-4-12(16)10(14)6-8/h1-6H,15-16H2
<b>InchiKey:</b>	HUWXDEQWWKGHVR-UHFFFAOYSA-N
<b>Formula:</b>	C12H10Cl2N2
<b>SMILES:</b>	<chem>Nc1ccc(-c2ccc(N)c(Cl)c2)cc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	253.13
<b>CAS:</b>	91-94-1

## Physical Properties

Property code	Value	Unit	Source
gf	345.50	kJ/mol	Joback Method
hf	172.27	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-4.92		Aqueous Solubility Prediction Method
logp	3.825		Crippen Method

mvol	176.860	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	395.30		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	395.30		NIST Webbook
rinpol	2463.00		NIST Webbook
rinpol	2416.64		NIST Webbook
rinpol	2416.64		NIST Webbook
tb	767.16	K	Joback Method
tc	1037.29	K	Joback Method
tf	405.65	K	Aqueous Solubility Prediction Method
vc	0.647	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.72	J/mol×K	767.16	Joback Method
cpg	441.78	J/mol×K	812.18	Joback Method
cpg	451.82	J/mol×K	857.20	Joback Method
cpg	460.90	J/mol×K	902.23	Joback Method
cpg	469.11	J/mol×K	947.25	Joback Method
cpg	476.50	J/mol×K	992.27	Joback Method
cpg	483.14	J/mol×K	1037.29	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C91941&Units=SI>

## Legend

**cpg:** Ideal gas heat capacity

<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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