

# p-chlorobenzylidene-(4-bromophenyl)-amine

**Inchi:** InChI=1S/C13H9BrClN/c14-11-3-7-13(8-4-11)16-9-10-1-5-12(15)6-2-10/h1-9H/b16-9+  
**InchiKey:** TXWQGAMPPNBAPT-CXUHLZMHS-A-N  
**Formula:** C13H9BrClN  
**SMILES:** Clc1ccc(C=Nc2ccc(Br)cc2)cc1  
**Mol. weight [g/mol]:** 294.57

## Physical Properties

Property code	Value	Unit	Source
hf	231.28	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.853		Crippen Method
mcvol	181.930	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	740.43	K	Joback Method
tc	1016.66	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159792&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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