

# p-bromobenzylidene-benzyl-amine

**Inchi:** InChI=1S/C14H12BrN/c15-14-8-6-13(7-9-14)11-16-10-12-4-2-1-3-5-12/h1-9,11H,10H2/b  
**InchiKey:** BXKIXPVEFBTGCW-LFIBNONCSA-N  
**Formula:** C14H12BrN  
**SMILES:** BrC1CCC(C=NCc2ccccc2)CC1  
**Mol. weight [g/mol]:** 274.16

## Physical Properties

Property code	Value	Unit	Source
hf	237.85	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.068		Crippen Method
mcvol	183.780	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	2143.00		NIST Webbook
tb	720.90	K	Joback Method
tc	987.99	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159618&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  
**log10ws:** 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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