

Benzenamine, 4-bromo-N-(phenylmethylene)-

Other names:	Aniline, N-benzylidene-p-bromo- Aniline, p-bromo-N-benzylidene- Benzylidene-p-bromoaniline N-Benzylidene-p-bromoaniline 1-Bromobezene,4-benzylidenamino Benzylidene-(4-bromophenyl)-amine
Inchi:	InChI=1S/C13H10BrN/c14-12-6-8-13(9-7-12)15-10-11-4-2-1-3-5-11/h1-10H
InchiKey:	DJGDQBWKJYPZEF-UHFFFAOYSA-N
Formula:	C13H10BrN
SMILES:	Brc1ccc(N=Cc2ccccc2)cc1
Mol. weight [g/mol]:	260.13
CAS:	780-20-1

Physical Properties

Property code	Value	Unit	Source
hf	258.49	kJ/mol	Joback Method
hvap	59.50	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.200		Crippen Method
mcvol	169.690	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	2086.00		NIST Webbook
tb	698.02	K	Joback Method
tc	971.97	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C780201&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{inpol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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