

1-Chlorobenzene, 4-(4-bromobenzylidenamino)-

Other names:	N-[(4-Bromophenyl)methylidene]-4-chloroaniline p-Bromobenzylidene-(4-chlorophenyl)-amine Benzenamine, N-[(4-bromophenyl)methylene]-4-chloro-
Inchi:	InChI=1S/C13H9BrClN/c14-11-3-1-10(2-4-11)9-16-13-7-5-12(15)6-8-13/h1-9H
InchiKey:	HYGUYDRZPYYAMJ-UHFFFAOYSA-N
Formula:	C13H9BrClN
SMILES:	Clc1ccc(N=Cc2ccc(Br)cc2)cc1
Mol. weight [g/mol]:	294.57
CAS:	55327-54-3

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
mvol	181.930	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	2289.00		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=C55327543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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