

1-BROMOBENZENE, 4-(4-BROMOBENZYLIDENEAMINO)-

Other names:	p-bromobenzylidene-(4-bromophenyl)-amine
Inchi:	InChI=1S/C13H9Br2N/c14-11-3-1-10(2-4-11)9-16-13-7-5-12(15)6-8-13/h1-9H
InchiKey:	XHEOIZWWHIMMFR-UHFFFAOYSA-N
Formula:	C13H9Br2N
SMILES:	<chem>BrC1CCC(C=Nc2ccc(Br)cc2)CC1</chem>
Mol. weight [g/mol]:	339.03

Physical Properties

Property code	Value	Unit	Source
hf	291.49	kJ/mol	Cheméo Relay (1.0)
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-5.66		Cheméo Relay (1.0)
logp	4.962		Crippen Method
mcvol	187.190	ml/mol	McGowan Method
tb	651.36	K	Cheméo Relay (1.0)
tf	410.17	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U221929&Units=SI
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
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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