

p-methylbenzylidene-(4-bromophenyl)-amine

Inchi:	InChI=1S/C14H12BrN/c1-11-2-4-12(5-3-11)10-16-14-8-6-13(15)7-9-14/h2-10H,1H3/b16-
InchiKey:	XTXVKVRGDHSVKS-MHWRWJLKSA-N
Formula:	C14H12BrN
SMILES:	<chem>Cc1ccc(C=Nc2ccc(Br)cc2)cc1</chem>
Mol. weight [g/mol]:	274.16

Physical Properties

Property code	Value	Unit	Source
hf	226.38	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.508		Crippen Method
mcvol	183.780	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2202.00		NIST Webbook
tb	725.88	K	Joback Method
tc	993.77	K	Joback Method

Sources

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=R160262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp:	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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