

N-(4-Bromobenzylidene)-p-toluidine

Other names:	N-[(4-Bromophenyl)methylidene]-4-methylaniline p-Bromobenzylidene-(4-methylphenyl)-amine
Inchi:	InChI=1S/C14H12BrN/c1-11-2-8-14(9-3-11)16-10-12-4-6-13(15)7-5-12/h2-10H,1H3
InchiKey:	JDEZSMCWSDUUAM-UHFFFAOYSA-N
Formula:	C14H12BrN
SMILES:	<chem>Cc1ccc(N=Cc2ccc(Br)cc2)cc1</chem>
Mol. weight [g/mol]:	274.16
CAS:	39128-27-3

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	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	725.88	K	Joback Method
tc	993.77	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39128273&Units=SI
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

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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