

p-bromobenzylidene-(3-methoxyphenyl)-amine

Inchi:	InChI=1S/C14H12BrNO/c1-17-14-4-2-3-13(9-14)16-10-11-5-7-12(15)8-6-11/h2-10H,1H3
InchiKey:	GHMNCILIZXKUJS-UHFFFAOYSA-N
Formula:	C14H12BrNO
SMILES:	COc1cccc(N=Cc2ccc(Br)cc2)c1
Mol. weight [g/mol]:	290.15

Physical Properties

Property code	Value	Unit	Source
hf	94.16	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.208		Crippen Method
mcvol	189.650	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
tb	748.30	K	Joback Method
tc	1011.19	K	Joback Method

Sources

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=R159529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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