

p-methoxybenzylidene-(3-bromophenyl)-amine

Inchi: InChI=1S/C14H12BrNO/c1-17-14-7-5-11(6-8-14)10-16-13-4-2-3-12(15)9-13/h2-10H,1H3
InchiKey: MHRKDSRHEAVPDU-UHFFFAOYSA-N
Formula: C14H12BrNO
SMILES: COc1ccc(C=Nc2ccccc(Br)c2)cc1
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	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	748.30	K	Joback Method
tc	1011.19	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159965&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
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

Latest version available from:

<https://www.cheméo.com/cid/48-327-6/p-methoxybenzylidene-3-bromophenyl-amine.pdf>

Generated by Cheméo on 2024-04-19 02:11:26.822751014 +0000 UTC m=+15781935.743328325.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.