

p-methylbenzylidene-(3-bromophenyl)-amine

Inchi: InChI=1S/C14H12BrN/c1-11-5-7-12(8-6-11)10-16-14-4-2-3-13(15)9-14/h2-10H,1H3
InchiKey: JOVMSELNSBEJTQ-UHFFFAOYSA-N
Formula: C14H12BrN
SMILES: Cc1ccc(C=Nc2cccc(Br)c2)cc1
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
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=R160202&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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