Benzylidene-(3-bromophenyl)-amine

Inchi: InChI=1S/C13H10BrN/c14-12-7-4-8-13(9-12)15-10-11-5-2-1-3-6-11/h1-10H/b15-10+
InchiKey: VDPUMIMWQUCITF-XNTDXEJSSA-N
Formula: C13H10BrN
SMILES: Brc1cccc(N=Cc2ccccc2)c1
Mol. weight [g/mol]: 260.13

Physical Properties

Property code	Value	Unit	Source
hf	258.49	kJ/mol	Joback Method
hvap	59.50	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.200		Crippen Method
mcvol	169.690	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	698.02	K	Joback Method
tc	971.97	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R158353&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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