

p-chlorobenzylidene-(3-bromophenyl)-amine

Inchi: InChI=1S/C13H9BrClN/c14-11-2-1-3-13(8-11)16-9-10-4-6-12(15)7-5-10/h1-9H
InchiKey: IQFXAIBPVAMQGX-UHFFFAOYSA-N
Formula: C13H9BrClN
SMILES: Clc1ccc(C=Nc2cccc(Br)c2)cc1
Mol. weight [g/mol]: 294.57

Physical Properties

Property code	Value	Unit	Source
hf	231.28	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.853		Crippen Method
mcvol	181.930	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinsol	2277.00		NIST Webbook
tb	740.43	K	Joback Method
tc	1016.66	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=R159732&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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