

Benzylidene-(3-chlorophenyl)-amine

Inchi: InChI=1S/C13H10ClN/c14-12-7-4-8-13(9-12)15-10-11-5-2-1-3-6-11/h1-10H
InchiKey: ZEXWWDRAHMCQOE-UHFFFAOYSA-N
Formula: C13H10ClN
SMILES: Clc1cccc(N=Cc2ccccc2)c1
Mol. weight [g/mol]: 215.68

Physical Properties

Property code	Value	Unit	Source
hf	216.42	kJ/mol	Joback Method
hvap	57.45	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.091		Crippen Method
mcvol	164.430	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	669.29	K	Joback Method
tc	934.27	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158368&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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