

N-Phenyl-N'-4-chlorophenylformamidine

Inchi: InChI=1S/C13H11ClN2/c14-11-6-8-13(9-7-11)16-10-15-12-4-2-1-3-5-12/h1-10H,(H,15,16)
InchiKey: UJQBEQAGNXOMOJ-UHFFFAOYSA-N
Formula: C13H11ClN2
SMILES: Clc1ccc(N=CNc2ccccc2)cc1
Mol. weight [g/mol]: 230.69

Physical Properties

Property code	Value	Unit	Source
hf	269.89	kJ/mol	Joback Method
hvap	63.88	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.112		Crippen Method
mcvol	174.410	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	719.46	K	Joback Method
tc	979.91	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=R161849&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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