

N,N-Dimethyl-N'-(3-chlorophenyl)-benzamidine

Inchi:	InChI=1S/C15H15ClN2/c1-18(2)15(12-7-4-3-5-8-12)17-14-10-6-9-13(16)11-14/h3-11H,1H
InchiKey:	CUYBJVVJAGGNAH-BMRADRMJSA-N
Formula:	C15H15ClN2
SMILES:	CN(C)C(=Nc1cccc(Cl)c1)c1ccccc1
Mol. weight [g/mol]:	258.75

Physical Properties

Property code	Value	Unit	Source
hf	232.88	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.980		Crippen Method
mcpvol	202.590	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	727.37	K	Joback Method
tc	979.92	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158615&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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