

# N,N-Dimethyl-N'-(4-chlorophenyl)-isobutyramidine

**Inchi:** InChI=1S/C12H17ClN2/c1-9(2)12(15(3)4)14-11-7-5-10(13)6-8-11/h5-9H,1-4H3  
**InchiKey:** XOUIRBMVWKUAPO-UHFFFAOYSA-N  
**Formula:** C12H17ClN2  
**SMILES:** CC(C)C(=Nc1ccc(Cl)cc1)N(C)C  
**Mol. weight [g/mol]:** 224.73

## Physical Properties

Property code	Value	Unit	Source
hf	52.99	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.588		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	631.61	K	Joback Method
tc	857.79	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=R162491&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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