

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

Inchi: InChI=1S/C12H17ClN2/c1-9(2)12(15(3)4)14-11-7-5-6-10(13)8-11/h5-9H,1-4H3/b14-12+
InchiKey: DZZGRYBMPQYPNY-WYMLVPIESA-N
Formula: C12H17ClN2
SMILES: CC(C)C(=Nc1cccc(Cl)c1)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	1740.00		NIST Webbook
tb	631.61	K	Joback Method
tc	857.79	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162377&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

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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