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

Inchi: InChI=1S/C11H15ClN2/c1-4-11(14(2)3)13-10-7-5-6-9(12)8-10/h5-8H,4H2,1-3H3/b13-11+
InchiKey: WJYPUACTLIXWJR-ACCUITESSA-N
Formula: C11H15ClN2
SMILES: CCC(=Nc1cccc(Cl)c1)N(C)C
Mol. weight [g/mol]: 210.70

Physical Properties

Property code	Value	Unit	Source
hf	78.91	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.342		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1713.00		NIST Webbook
rinpol	1713.00		NIST Webbook
tb	609.17	K	Joback Method
tc	834.93	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R161894&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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