

N'-(3-chloro-phenyl)-N,N-dimethyl-acetamide

Inchi: InChI=1S/C10H13ClN2/c1-8(13(2)3)12-10-6-4-5-9(11)7-10/h4-7H,1-3H3/b12-8+
InchiKey: RYQOCMLDBOZFRD-XYOKQWHBSA-N
Formula: C10H13ClN2
SMILES: CC(=Nc1cccc(Cl)c1)N(C)C
Mol. weight [g/mol]: 196.68

Physical Properties

Property code	Value	Unit	Source
hf	99.55	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.951		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1666.00		NIST Webbook
tb	586.29	K	Joback Method
tc	816.46	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R153234&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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