

N,N-Dimethyl-N'-(3-methylphenyl)-p-chlorobenzamide

Inchi: InChI=1S/C16H17ClN2/c1-12-5-4-6-15(11-12)18-16(19(2)3)13-7-9-14(17)10-8-13/h4-11H
InchiKey: WCPTYUIXJNTXBW-FBMGVBCBSA-N
Formula: C16H17ClN2
SMILES: Cc1cccc(N=C(c2ccc(Cl)cc2)N(C)C)c1
Mol. weight [g/mol]: 272.77

Physical Properties

Property code	Value	Unit	Source
hf	200.77	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.288		Crippen Method
mcvol	216.680	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2061.00		NIST Webbook
tb	755.23	K	Joback Method
tc	1003.10	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158744&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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