

N,N-Dimethyl-2-phenyl-N'-(3-chlorophenyl)-acetar

Inchi: InChI=1S/C16H17ClN2/c1-19(2)16(11-13-7-4-3-5-8-13)18-15-10-6-9-14(17)12-15/h3-10,
InchiKey: GVOICEOGUAGKBS-FBMGVBCBSA-N
Formula: C16H17ClN2
SMILES: CN(C)C(Cc1ccccc1)=Nc1cccc(Cl)c1
Mol. weight [g/mol]: 272.77

Physical Properties

Property code	Value	Unit	Source
hf	212.24	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.174		Crippen Method
mcvol	216.680	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	750.25	K	Joback Method
tc	997.36	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162139&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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