N,N-Dimethyl-N'-(4-methoxyphenyl)-p-chlorobenz

Inchi: InChI=1S/C16H17ClN2O/c1-19(2)16(12-4-6-13(17)7-5-12)18-14-8-10-15(20-3)11-9-14/h
InchiKey: BBPVWNLNJGTNDG-UHFFFAOYSA-N
Formula: C16H17ClN2O
SMILES: COc1ccc(/N=C(\c2ccc(Cl)cc2)N(C)C)cc1
Mol. weight [g/mol]: 288.78

Physical Properties

Property code	Value	Unit	Source
hvap	92.80	kJ/mol	Cheméo Relay (1.0)
ie	7.07	eV	Cheméo Relay (1.0)
log10ws	-4.58		Cheméo Relay (1.0)
logp	3.989		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
rinpol	2224.00		NIST Webbook
tb	659.50	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R158942&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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