

N''-(4-methoxy-phenyl)-N,N,N',N'-tetramethyl-guanidine

Inchi:	InChI=1S/C12H19N3O/c1-14(2)12(15(3)4)13-10-6-8-11(16-5)9-7-10/h6-9H,1-5H3
InchiKey:	IHEVQCXBONXGO-UHFFFAOYSA-N
Formula:	C12H19N3O
SMILES:	COc1ccc(N=C(N(C)C)N(C)C)cc1
Mol. weight [g/mol]:	221.30

Physical Properties

Property code	Value	Unit	Source
hf	9.32	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.806		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	629.48	K	Joback Method
tc	841.84	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153076&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

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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