

N,N-Dimethyl-N'-(3-methoxyphenyl)-benzamidine

Inchi:	InChI=1S/C16H18N2O/c1-18(2)16(13-8-5-4-6-9-13)17-14-10-7-11-15(12-14)19-3/h4-12H
InchiKey:	FEQSEUNJZRBLPJ-WUKNDPDISA-N
Formula:	C16H18N2O
SMILES:	COc1ccccc(N=C(c2ccccc2)N(C)C)c1
Mol. weight [g/mol]:	254.33

Physical Properties

Property code	Value	Unit	Source
hf	95.76	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.335		Crippen Method
mcvol	210.310	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	2048.00		NIST Webbook
tb	735.24	K	Joback Method
tc	976.42	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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