

N,N-Dimethyl-N'-(3-bromophenyl)-p-methoxybenz

Inchi:	InChI=1S/C16H17BrN2O/c1-19(2)16(12-7-9-15(20-3)10-8-12)18-14-6-4-5-13(17)11-14/h
InchiKey:	XKEQVFLSXBIRAV-FBMGVBCBSA-N
Formula:	C16H17BrN2O
SMILES:	COc1ccc(C(=Nc2cccc(Br)c2)N(C)C)cc1
Mol. weight [g/mol]:	333.22

Physical Properties

Property code	Value	Unit	Source
hf	110.62	kJ/mol	Joback Method
hvap	71.37	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.098		Crippen Method
mcvol	227.810	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2320.00		NIST Webbook
tb	806.38	K	Joback Method
tc	1057.65	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R158591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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