

N,N-Dimethyl-N'-(4-bromophenyl)-p-methoxybenz

Inchi: InChI=1S/C16H17BrN2O/c1-19(2)16(12-4-10-15(20-3)11-5-12)18-14-8-6-13(17)7-9-14/h
InchiKey: BDSIMZMKGLVABN-UHFFFAOYSA-N
Formula: C16H17BrN2O
SMILES: COc1ccc(C(=Nc2ccc(Br)cc2)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	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	806.38	K	Joback Method
tc	1057.65	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158833&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
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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