

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

Inchi: InChI=1S/C16H17BrN2/c1-12-7-9-13(10-8-12)16(19(2)3)18-15-6-4-5-14(17)11-15/h4-11H
InchiKey: CAHOETBWTBKYIK-FBMGVBCBSA-N
Formula: C16H17BrN2
SMILES: Cc1ccc(C(=Nc2cccc(Br)c2)N(C)C)cc1
Mol. weight [g/mol]: 317.22

Physical Properties

Property code	Value	Unit	Source
hf	242.84	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.397		Crippen Method
mcvol	221.940	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	783.96	K	Joback Method
tc	1039.31	K	Joback Method

Sources

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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158600&Units=SI>

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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