

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

Inchi:	InChI=1S/C15H14BrClN2/c1-19(2)15(11-6-8-13(17)9-7-11)18-14-5-3-4-12(16)10-14/h3-1
InchiKey:	NNQMSJUNDWWKCL-UHFFFAOYSA-N
Formula:	C15H14BrClN2
SMILES:	CN(C)C(=Nc1cccc(Br)c1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	337.64

Physical Properties

Property code	Value	Unit	Source
hf	247.74	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.742		Crippen Method
mcvol	220.090	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2293.00		NIST Webbook
tb	798.51	K	Joback Method
tc	1061.15	K	Joback Method

Sources

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=R158586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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