N,N-Dimethyl-2-phenyl-N'-(3-bromophenyl)-acetar

Inchi: InChI=1S/C16H17BrN2/c1-19(2)16(11-13-7-4-3-5-8-13)18-15-10-6-9-14(17)12-15/h3-10,
InchiKey: HQLVJGXCPSQFLW-FBMGVBCBSA-N
Formula: C16H17BrN2
SMILES: CN(C)C(Cc1ccccc1)=Nc1cccc(Br)c1
Mol. weight [g/mol]: 317.22

Physical Properties

Property code	Value	Unit	Source
hf	254.31	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.283		Crippen Method
mcvol	221.940	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	2351.00		NIST Webbook
rinpol	2351.00		NIST Webbook
tb	778.98	K	Joback Method
tc	1033.60	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R162124&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