

N'-(3-bromo-phenyl)-N,N-dimethyl-acetamide

Inchi: InChI=1S/C10H13BrN2/c1-8(13(2)3)12-10-6-4-5-9(11)7-10/h4-7H,1-3H3/b12-8+
InchiKey: KKOWZUCUYFUHBH-XYOKQWHBSA-N
Formula: C10H13BrN2
SMILES: CC(=Nc1cccc(Br)c1)N(C)C
Mol. weight [g/mol]: 241.13

Physical Properties

Property code	Value	Unit	Source
hf	141.62	kJ/mol	Joback Method
hvap	52.66	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.061		Crippen Method
mcvol	161.160	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	615.02	K	Joback Method
tc	854.39	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R153214&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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