p-bromobenzylidene-(3-nitrophenyl)-amine

Inchi: InChI=1S/C13H9BrN2O2/c14-11-6-4-10(5-7-11)9-15-12-2-1-3-13(8-12)16(17)18/h1-9H
InchiKey: ZFDQTTNNOHUVCU-UHFFFAOYSA-N
Formula: C13H9BrN2O2
SMILES: O=[N+]([O-])c1cccc(N=Cc2ccc(Br)cc2)c1
Mol. weight [g/mol]: 305.13

Physical Properties

Property code	Value	Unit	Source
hf	236.26	kJ/mol	Joback Method
hvap	76.75	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.108		Crippen Method
mcvol	187.110	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	2526.00		NIST Webbook
tb	854.84	K	Joback Method
tc	1144.44	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R159549&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