p-Nitrobenzylidene tert-butylamine

Other names: tert-Butyl-(4-nitro-benzylidene)-amine
Inchi: InChI=1S/C11H14N2O2/c1-11(2,3)12-8-9-4-6-10(7-5-9)13(14)15/h4-8H,1-3H3
InchiKey: BZCRPTQYJYKZDH-UHFFFAOYSA-N
Formula: C11H14N2O2
SMILES: CC(C)(C)N=Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 206.24
CAS: 718-36-5

Physical Properties

Property code	Value	Unit	Source
chs	-6287.70 ± 1.00	kJ/mol	NIST Webbook
hf	49.40 ± 3.60	kJ/mol	NIST Webbook
hfs	-41.70 ± 1.80	kJ/mol	NIST Webbook
hsub	91.10 ± 3.10	kJ/mol	NIST Webbook
hsub	91.10 ± 3.10	kJ/mol	NIST Webbook
hvap	61.63	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.812		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	708.03	K	Joback Method
tc	966.32	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=C718365&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature