

tert-Butyl-(4-nitro-benzylidene)-amine

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]:	206.25

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
ie	9.16	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.812		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
tb	551.20	K	Cheméo Relay (1.0)
tf	373.24	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C718365&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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