Benzylidene-(4-nitrophenyl)-amine

Other names: Benzenamine, 4-nitro-N-(phenylmethylene)-
Inchi: InChI=1S/C13H10N2O2/c16-15(17)13-8-6-12(7-9-13)14-10-11-4-2-1-3-5-11/h1-10H
InchiKey: NYJOAZXGKLCRSV-UHFFFAOYSA-N
Formula: C13H10N2O2
SMILES: O=[N+]([O-])c1ccc(N=Cc2ccccc2)cc1
Mol. weight [g/mol]: 226.23
CAS: 69173-79-1

Physical Properties

Property code	Value	Unit	Source
hf	221.40	kJ/mol	Joback Method
hvap	69.65	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.76	eV	NIST Webbook
log10ws	-3.99		Crippen Method
logp	3.345		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	2259.00		NIST Webbook
tb	783.70	K	Joback Method
tc	1064.35	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=C69173791&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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