Benzenamine, 3-nitro-N-(phenylmethylene)-

Other names:	Aniline, N-benzylidene-m-nitro-
	Benzal-m-nitroaniline
	Benzylidene-m-nitroaniline
	N-Benzylidene-m-nitroaniline
	3-Nitro-N-(benzylidene)aniline
	N-Benzylidene-3-nitroaniline
	Benzylidene-(3-nitrophenyl)-amine
Inchi:	InChI=1S/C13H10N2O2/c16-15(17)13-8-4-7-12(9-13)14-10-11-5-2-1-3-6-11/h1-10H
InchiKey:	HFGFPUPROHHWFT-UHFFFAOYSA-N
Formula:	C13H10N2O2
SMILES:	O=[N+]([O-])c1cccc(N=Cc2ccccc2)c1
Mol. weight [g/mol]:	226.23
CAS:	5341-44-6

Physical Properties

Property code	Value	Unit	Source
hf	221.40	kJ/mol	Joback Method
hvap	69.65	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.345		Crippen Method
mcvol	169.610	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	2212.00		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=C5341446&Units=SI

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