

# Benzenamine,N-[(3-methylphenyl)methylene]-4-ni

Inchi:	InChI=1S/C14H12N2O2/c1-11-3-2-4-12(9-11)10-15-13-5-7-14(8-6-13)16(17)18/h2-10H,1
InchiKey:	VQCDHUITEKSJND-XNTDXEJSSA-N
Formula:	C14H12N2O2
SMILES:	Cc1cccc(C=Nc2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]:	240.26
CAS:	62453-03-6

## Physical Properties

Property code	Value	Unit	Source
hf	189.29	kJ/mol	Joback Method
hvap	72.54	kJ/mol	Joback Method
ie	8.58	eV	NIST Webbook
log10ws	-4.46		Crippen Method
logp	3.654		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
tb	811.56	K	Joback Method
tc	1085.88	K	Joback Method

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C62453036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C62453036&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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