

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

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=C62453036&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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