

Methanamine, N-(phenylmethylene)-, N-oxide

Other names:	Nitrone, N-methyl-«alpha»-phenyl- «alpha»-Phenyl-N-methylnitrone C-Phenyl-N-methylnitrone N-Benzylidenemethylamine N-oxide N-Methyl-«alpha»-phenylnitrone N-Methyl-C-phenylnitrone N-Methylphenylnitrone Methylamine, N-benzylidene-, N-oxide Benzylidenemethylamine N-oxide N-(Phenylmethylene)methanamine N-oxide
Inchi:	InChI=1S/C8H9NO/c1-9(10)7-8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	AKVBBQCAQAJLKM-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	<chem>C[N+](=[O-])=Cc1ccccc1</chem>
Mol. weight [g/mol]:	135.16
CAS:	3376-23-6

Physical Properties

Property code	Value	Unit	Source
ie	8.01	eV	NIST Webbook
ie	8.08 ± 0.05	eV	NIST Webbook
ie	8.01	eV	NIST Webbook
ie	7.89	eV	NIST Webbook
ie	8.01 ± 0.02	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	1.246		Crippen Method
mcvol	111.370	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3376236&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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