

Benzonitrile, N-oxide

Other names:	Benzonitrile oxide Phenylnitrile oxide
Inchi:	InChI=1S/C7H5NO/c9-8-6-7-4-2-1-3-5-7/h1-5H
InchiKey:	QUNPTMGXSSDZHZ-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	[O-][N+]#Cc1ccccc1
Mol. weight [g/mol]:	119.12
CAS:	873-67-6

Physical Properties

Property code	Value	Unit	Source
ie	8.96 ± 0.02	eV	NIST Webbook
log10ws	-5.17		Crippen Method
logp	1.865		Crippen Method
mcvol	92.980	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C873676&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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