Quinoline, 1-oxide

Other names:	Quinoline oxide
	Quinoline N-oxide
Inchi:	InChI=1S/C9H7NO/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	GIIWGCBLYNDKBO-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	[O-][n+]1cccc2ccccc21
Mol. weight [g/mol]:	145.16
CAS:	1613-37-2

Physical Properties

Property code	Value	Unit	Source
affp	943.30	kJ/mol	NIST Webbook
basg	910.80	kJ/mol	NIST Webbook
ie	8.00 ± 0.05	eV	NIST Webbook
log10ws	-4.80		Crippen Method
logp	1.473		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume