

Isoquinoline, 2-oxide

Other names:	Isoquinoline oxide Isoquinoline N-oxide isoquinolin-N-oxide
Inchi:	InChI=1S/C9H7NO/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey:	RZIAABRFQASVSW-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	[O-][n+]1ccc2ccccc2c1
Mol. weight [g/mol]:	145.16
CAS:	1532-72-5

Physical Properties

Property code	Value	Unit	Source
ie	7.90	eV	NIST Webbook
ie	7.98 ± 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=C1532725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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