

Isoquinolinium,3,4-dihydro-2-hydroxy-hydroxide,inner salt

InChI:	InChI=1S/C9H9NO/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-4,7H,5-6H2
InChIKey:	AXQPWUAAOXVGOR-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	[O-][N+]1=Cc2ccccc2CC1
Mol. weight [g/mol]:	147.17
CAS:	65194-03-8

Physical Properties

Property code	Value	Unit	Source
ie	7.81	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.172		Crippen Method
mcvol	114.600	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=C65194038&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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