

Quinoxaline, 1-oxide

Other names:	Quinoxaline mono-N-oxide Quinoxaline monooxide Quinoxaline N-oxide Quinoxaline, N-monooxide 4-Quinoxaline mono-N-oxide
Inchi:	InChI=1S/C8H6N2O/c11-10-6-5-9-7-3-1-2-4-8(7)10/h1-6H
InchiKey:	OARGFWQSVACNCO-UHFFFAOYSA-N
Formula:	C8H6N2O
SMILES:	[O-][n+]1ccnc2ccccc21
Mol. weight [g/mol]:	146.15
CAS:	6935-29-1

Physical Properties

Property code	Value	Unit	Source
ie	8.62 ± 0.05	eV	NIST Webbook
log10ws	-4.57		Crippen Method
logp	0.868		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6935291&Units=SI
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

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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