

2-Methyl-8-nitroindolizine

Inchi:	InChI=1S/C9H8N2O2/c1-7-5-9-8(11(12)13)3-2-4-10(9)6-7/h2-6H,1H3
InchiKey:	RVNQZWLKCLWQOQ-UHFFFAOYSA-N
Formula:	C9H8N2O2
SMILES:	<chem>Cc1cc2c([N+](=O)[O-])cccn2c1</chem>
Mol. weight [g/mol]:	176.17
CAS:	60891-78-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.156		Crippen Method
mcvol	126.150	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=C60891783&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/27-901-1/2-Methyl-8-nitroindolizine.pdf>

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