

Nitroxoline, acetate

Inchi:	InChI=1S/C11H8N2O4/c1-7(14)17-10-5-4-9(13(15)16)8-3-2-6-12-11(8)10/h2-6H,1H3
InchiKey:	WVWNMQHUCFCDDM-UHFFFAOYSA-N
Formula:	C11H8N2O4
SMILES:	CC(=O)Oc1ccc([N+](=O)[O-])c2cccnc12
Mol. weight [g/mol]:	232.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.068		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U393993&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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