Quinoline, 4-nitro-, 1-oxide

Other names:	Nitrochin
	4-Nitroquinoline oxide
	4-Nitroquinoline N-oxide
	4-Nitroquinoline 1-oxide
	4-NQO
	4-Nitrochinolin N-oxid
	NSC 19645
Inchi:	InChI=1S/C9H6N2O3/c12-10-6-5-9(11(13)14)7-3-1-2-4-8(7)10/h1-6H
InchiKey:	YHQDZJICGQWFHK-UHFFFAOYSA-N
Formula:	C9H6N2O3
SMILES:	O=[N+]([O-])c1cc[n+]([O-])c2ccccc12
Mol. weight [g/mol]:	190.16
CAS:	56-57-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	1.381		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
rinpol	330.31		NIST Webbook
rinpol	330.82		NIST Webbook
rinpol	331.55		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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