

2,4-Quinolinediol, 3-nitroso- (keto form)

Inchi:	InChI=1S/C9H6N2O3/c12-8-5-3-1-2-4-6(5)10-9(13)7(8)11-14/h1-4H,(H2,10,12,13)
InchiKey:	QOWGKOOAVPYSPT-UHFFFAOYSA-N
Formula:	C9H6N2O3
SMILES:	O=Nc1c(O)c2ccccc2[nH]c1=O
Mol. weight [g/mol]:	190.16
CAS:	99066-74-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	1.150		Crippen Method
mcvol	127.720	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=C99066747&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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