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/ci990307l
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