4-Nitro-5-hydroxy-1,2-dimethylindole

Inchi: InChI=1S/C10H10N2O3/c1-6-5-7-8(11(6)2)3-4-9(13)10(7)12(14)15/h3-5,13H,1-2H3
InchiKey: AAHRWLRCEUVGFY-UHFFFAOYSA-N
Formula: C10H10N2O3
SMILES: Cc1cc2c([N+](=O)[O-])c(O)ccc2n1C
Mol. weight [g/mol]: 206.20
CAS: 53918-86-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	2.101		Crippen Method
mcvol	146.110	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=C53918868&Units=SI

Legend

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