

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:	<chem>Cc1cc2c([N+](=O)[O-])c(O)ccc2n1C</chem>
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

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