

3-Hydroxy-6-methyl-2-nitropyridine

Other names:	6-Methyl-2-nitro-3-pyridinol 3-Pyridinol, 6-methyl-2-nitro- 6-methyl-2-nitropyridin-3-ol
Inchi:	InChI=1S/C6H6N2O3/c1-4-2-3-5(9)6(7-4)8(10)11/h2-3,9H,1H3
InchiKey:	WZMGQHIBXUAYGS-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	<chem>Cc1ccc(O)c([N+](=O)[O-])n1</chem>
Mol. weight [g/mol]:	154.12
CAS:	15128-90-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.004		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15128902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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