

2-Hydroxy-5-nitropyridine

Other names:	5-Nitro-2-hydroxypyridine 5-Nitro-2-pyridinol 5-Nitro-2-pyridinone 5-Nitro-2(1H)-pyridinone 5-Nitro-2-pyridone 5-Nitro-2(1H)-pyridone 2-Pyridinol, 5-nitro- 2(1H)-Pyridinone, 5-nitro- 5-nitropyridin-2-ol
Inchi:	InChI=1S/C5H4N2O3/c8-5-2-1-4(3-6-5)7(9)10/h1-3H,(H,6,8)
InchiKey:	XKWSQIMYNVLGBO-UHFFFAOYSA-N
Formula:	C5H4N2O3
SMILES:	O=c1ccc([N+](=O)[O-])c[nH]1
Mol. weight [g/mol]:	140.10
CAS:	5418-51-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	-0.199		Crippen Method
mcvol	90.820	ml/mol	McGowan Method

Sources

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=C5418519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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