

4-Methyl-3-nitropyridine

Inchi:	InChI=1S/C6H6N2O2/c1-5-2-3-7-4-6(5)8(9)10/h2-4H,1H3
InchiKey:	JLNRJMGYBKMDGI-UHFFFAOYSA-N
Formula:	C6H6N2O2
SMILES:	Cc1ccncc1[N+](=O)[O-]
Mol. weight [g/mol]:	138.12
CAS:	5832-44-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	1.298		Crippen Method
mcvol	99.040	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=C5832440&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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