4-Nitro-2-picoline N-oxide

Other names:	4-Nitro-2-methylpyridine N-oxide
	Pyridine, 2-methyl-4-nitro-, 1-oxide
	2-Methyl-4-nitropyridine 1-oxide
	2-Methyl-4-nitropyridine N-oxide
	4-Nitro-«alpha»-picoline N-oxide
	4-Nitro-2-methylpyridine 1-oxide
	2-Picoline, 4-nitro-, 1-oxide
	NSC 27962
Inchi:	InChI=1S/C6H6N2O3/c1-5-4-6(8(10)11)2-3-7(5)9/h2-4H,1H3
InchiKey:	FTTIAVRPJGCXAC-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	Cc1cc([N+](=O)[O-])cc[n+]1[O-]
Mol. weight [g/mol]:	154.12
CAS:	5470-66-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	0.537		Crippen Method
mcvol	104.910	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=C5470666&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume