

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:	<chem>Cc1cc([N+](=O)[O-])cc[n+][O-]</chem>
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/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/52-314-5/4-Nitro-2-picoline-N-oxide.pdf>

Generated by Cheméo on 2024-04-28 09:59:54.740552019 +0000 UTC m=+16587643.661129331.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.