

4-Nitro-3-picoline-N-oxide

Other names:	Pyridine, 3-methyl-4-nitro-, 1-oxide 3-Methyl-4-nitropyridine 1-oxide 3-Picoline, 4-nitro-, 1-oxide 4-Nitro-«beta»-picoline N-oxide 4-Nitro-3-methylpyridine N-oxide 4-Nitro-3-picoline 1-oxide 5-Methyl-4-nitropyridine N-oxide 3-Methyl-4-nitropyridine N-oxide NSC 168202 NSC 74203
Inchi:	InChI=1S/C6H6N2O3/c1-5-4-7(9)3-2-6(5)8(10)11/h2-4H,1H3
InchiKey:	SSOURMYKACOBIV-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	<chem>Cc1c[n+](O)ccc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	154.12
CAS:	1074-98-2

Physical Properties

Property code	Value	Unit	Source
hsub	106.70 ± 2.00	kJ/mol	NIST Webbook
log10ws	-4.13		Crippen Method
logp	0.537		Crippen Method
mvol	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=C1074982&Units=SI

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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