6-METHYL-2-NITRO-3-PYRIDINOL

Other names:	6-Methyl-2-nitro-3-pyridinol
	3-Pyridinol, 6-methyl-2-nitro-
	6-methyl-2-nitropyridin-3-ol
Inchi:	InChI=1S/C6H6N2O3/c1-4-2-3-5(9)6(7-4)8(10)11/h2-3,9H,1H3
InchiKey:	WZMGQHIBXUAYGS-UHFFFAOYSA-N
Formula:	C6H6N2O3
SMILES:	Cc1ccc(O)c([N+](=O)[O-])n1
Mol. weight [g/mol]:	154.13

Physical Properties

Property code	Value	Unit	Source
hvap	59.29	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
logp	1.004		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
tf	356.64	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15128902&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point